Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 01:39 am BST

PDB ID	:	8OH5 / pdb_00008oh5
EMDB ID	:	EMD-16878
Title	:	Cryo-EM structure of the electron bifurcating transhydrogenase StnABC complex from Sporomusa Ovata (state 2)
Authors	:	Kumar, A.; Kremp, F.; Mueller, V.; Schuller, J.M.
Deposited on	:	2023-03-20
Resolution	:	3.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

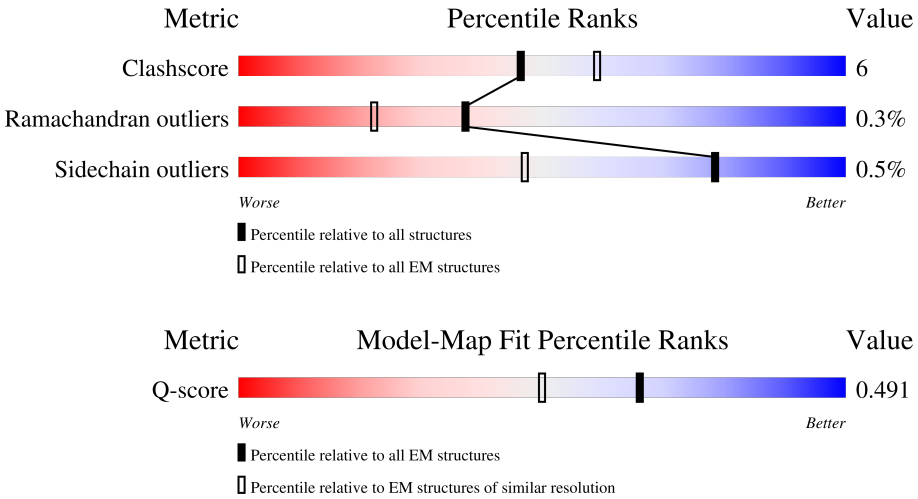
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	178	43% 65% 17% •• 16%
1	D	178	42% 65% 18% • 16%
1	G	178	42% 65% 18% •• 16%
1	J	178	42% 65% 18% • 16%

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Mol	Chain	Length	Quality of chain
2	B	584	47% 83% 17%
2	E	584	47% 83% 16%
2	H	584	47% 83% 17%
2	K	584	47% 83% 16%
3	C	1172	88% 12%
3	F	1172	88% 12%
3	I	1172	88% 12%
3	L	1172	87% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SF4	B	604	-	-	X	-
7	SF4	E	604	-	-	X	-
7	SF4	H	604	-	-	X	-
7	SF4	K	604	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 58624 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NAD-dependent formate dehydrogenase gamma subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	150	Total	C	N	O	S	0	0
			1118	717	182	212	7		
1	D	150	Total	C	N	O	S	0	0
			1118	717	182	212	7		
1	G	150	Total	C	N	O	S	0	0
			1118	717	182	212	7		
1	J	150	Total	C	N	O	S	0	0
			1118	717	182	212	7		

- Molecule 2 is a protein called NAD-reducing hydrogenase subunit HoxF.

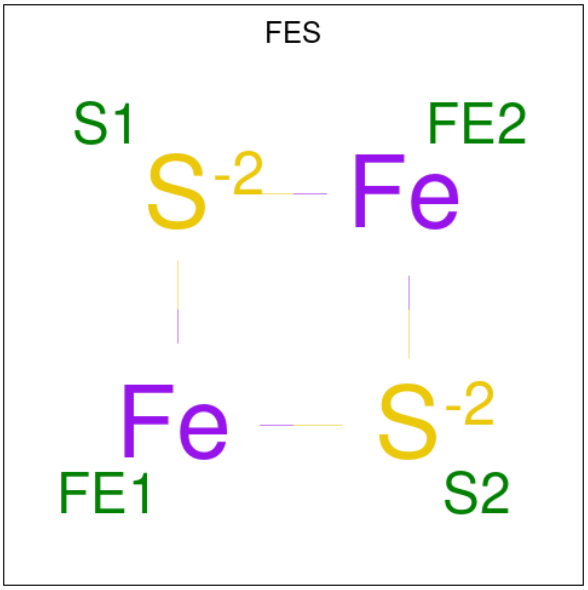
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	584	Total	C	N	O	S	0	0
			4431	2789	758	839	45		
2	E	584	Total	C	N	O	S	0	0
			4431	2789	758	839	45		
2	H	584	Total	C	N	O	S	0	0
			4431	2789	758	839	45		
2	K	584	Total	C	N	O	S	0	0
			4431	2789	758	839	45		

- Molecule 3 is a protein called Formate dehydrogenase-O, major subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1172	Total	C	N	O	S	0	0
			8846	5554	1522	1710	60		
3	F	1172	Total	C	N	O	S	0	0
			8846	5554	1522	1710	60		
3	I	1172	Total	C	N	O	S	0	0
			8846	5554	1522	1710	60		
3	L	1172	Total	C	N	O	S	0	0
			8846	5554	1522	1710	60		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled

as "Ligand of Interest" by depositor).



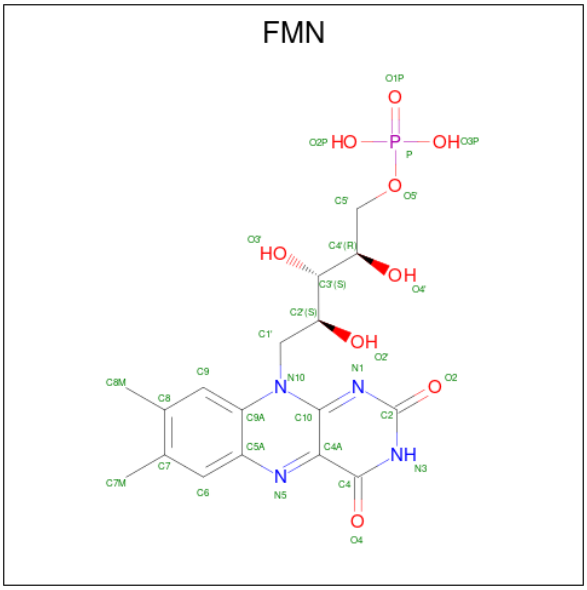
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Fe S 4 2 2	0
4	B	1	Total Fe S 4 2 2	0
4	C	1	Total Fe S 4 2 2	0
4	D	1	Total Fe S 4 2 2	0
4	E	1	Total Fe S 4 2 2	0
4	F	1	Total Fe S 4 2 2	0
4	G	1	Total Fe S 4 2 2	0
4	H	1	Total Fe S 4 2 2	0
4	I	1	Total Fe S 4 2 2	0
4	J	1	Total Fe S 4 2 2	0
4	K	1	Total Fe S 4 2 2	0
4	L	1	Total Fe S 4 2 2	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by

depositor).

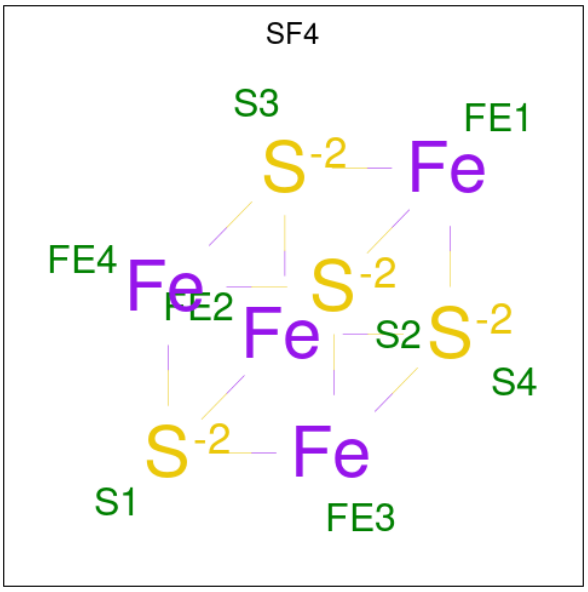
Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total Zn 1 1	0
5	E	1	Total Zn 1 1	0
5	H	1	Total Zn 1 1	0
5	K	1	Total Zn 1 1	0

- Molecule 6 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
6	B	1	Total C N O P 31 17 4 9 1	0
6	E	1	Total C N O P 31 17 4 9 1	0
6	H	1	Total C N O P 31 17 4 9 1	0
6	K	1	Total C N O P 31 17 4 9 1	0

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
7	B	1	Total Fe S 8 4 4	0
7	B	1	Total Fe S 8 4 4	0
7	B	1	Total Fe S 8 4 4	0
7	C	1	Total Fe S 8 4 4	0
7	C	1	Total Fe S 8 4 4	0
7	C	1	Total Fe S 8 4 4	0
7	C	1	Total Fe S 8 4 4	0
7	C	1	Total Fe S 8 4 4	0
7	C	1	Total Fe S 8 4 4	0
7	E	1	Total Fe S 8 4 4	0
7	E	1	Total Fe S 8 4 4	0
7	E	1	Total Fe S 8 4 4	0
7	F	1	Total Fe S 8 4 4	0
7	F	1	Total Fe S 8 4 4	0

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Mol	Chain	Residues	Atoms	AltConf
7	F	1	Total Fe S 8 4 4	0
7	F	1	Total Fe S 8 4 4	0
7	F	1	Total Fe S 8 4 4	0
7	F	1	Total Fe S 8 4 4	0
7	H	1	Total Fe S 8 4 4	0
7	H	1	Total Fe S 8 4 4	0
7	H	1	Total Fe S 8 4 4	0
7	I	1	Total Fe S 8 4 4	0
7	I	1	Total Fe S 8 4 4	0
7	I	1	Total Fe S 8 4 4	0
7	I	1	Total Fe S 8 4 4	0
7	I	1	Total Fe S 8 4 4	0
7	I	1	Total Fe S 8 4 4	0
7	K	1	Total Fe S 8 4 4	0
7	K	1	Total Fe S 8 4 4	0
7	K	1	Total Fe S 8 4 4	0
7	L	1	Total Fe S 8 4 4	0
7	L	1	Total Fe S 8 4 4	0
7	L	1	Total Fe S 8 4 4	0
7	L	1	Total Fe S 8 4 4	0
7	L	1	Total Fe S 8 4 4	0

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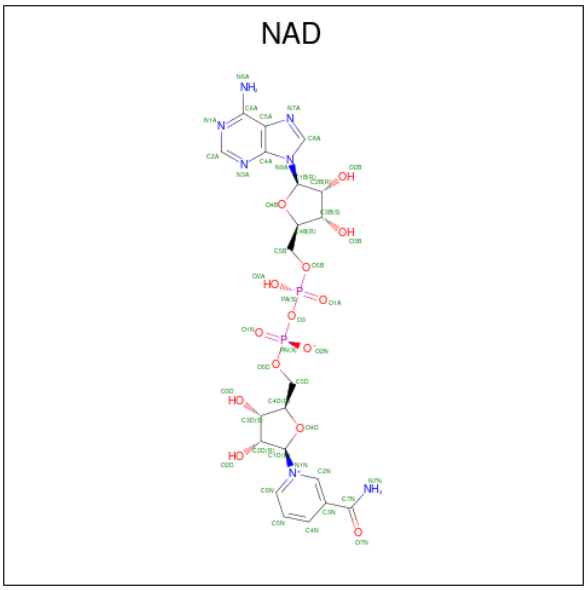
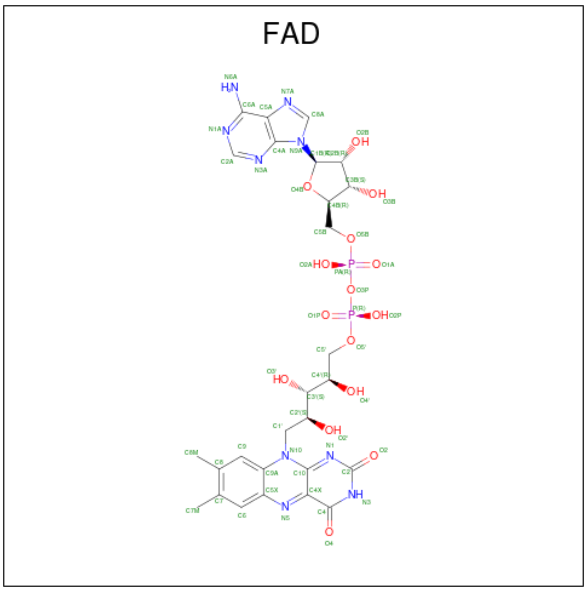
Mol	Chain	Residues	Atoms			AltConf
7	L	1	Total	Fe	S	0
			8	4	4	

- Molecule 8 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



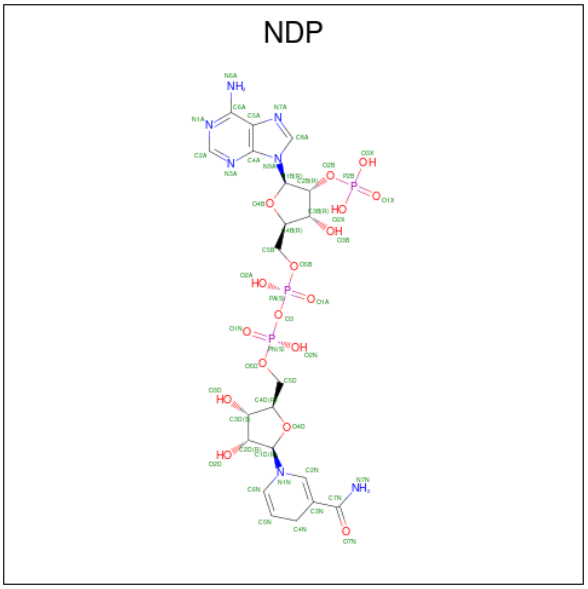
Mol	Chain	Residues	Atoms					AltConf
8	B	1	Total	C	N	O	P	0
			44	21	7	14	2	
8	E	1	Total	C	N	O	P	0
			44	21	7	14	2	
8	H	1	Total	C	N	O	P	0
			44	21	7	14	2	
8	K	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	C	1	Total	C	N	O	P	0
			53	27	9	15	2	
9	F	1	Total	C	N	O	P	0
			53	27	9	15	2	
9	I	1	Total	C	N	O	P	0
			53	27	9	15	2	
9	L	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 10 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



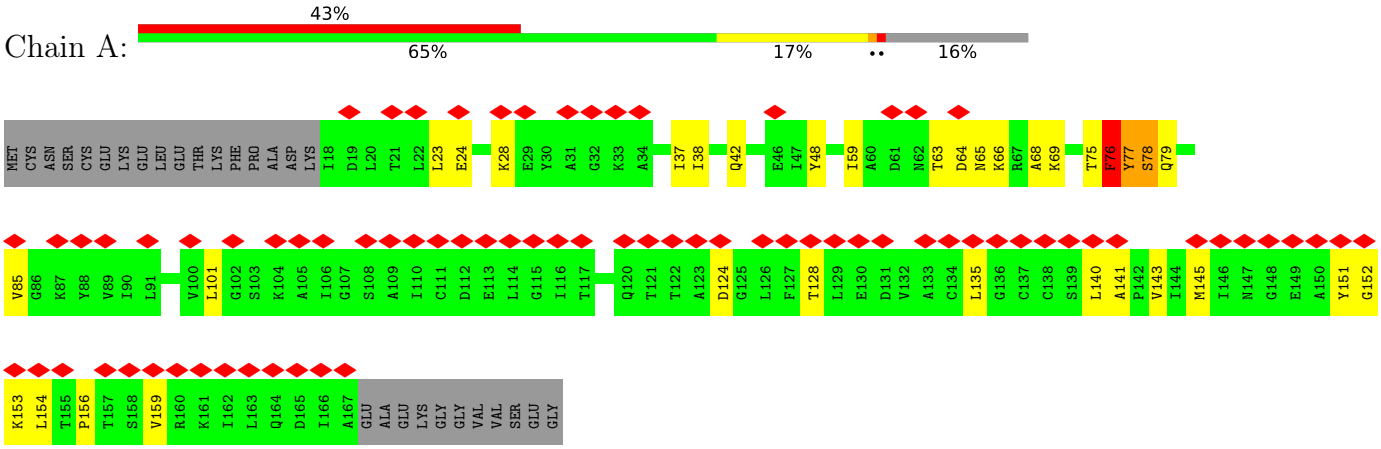
Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total	C	N	O	P	0
			48	21	7	17	3	
10	F	1	Total	C	N	O	P	0
			48	21	7	17	3	
10	I	1	Total	C	N	O	P	0
			48	21	7	17	3	
10	L	1	Total	C	N	O	P	0
			48	21	7	17	3	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

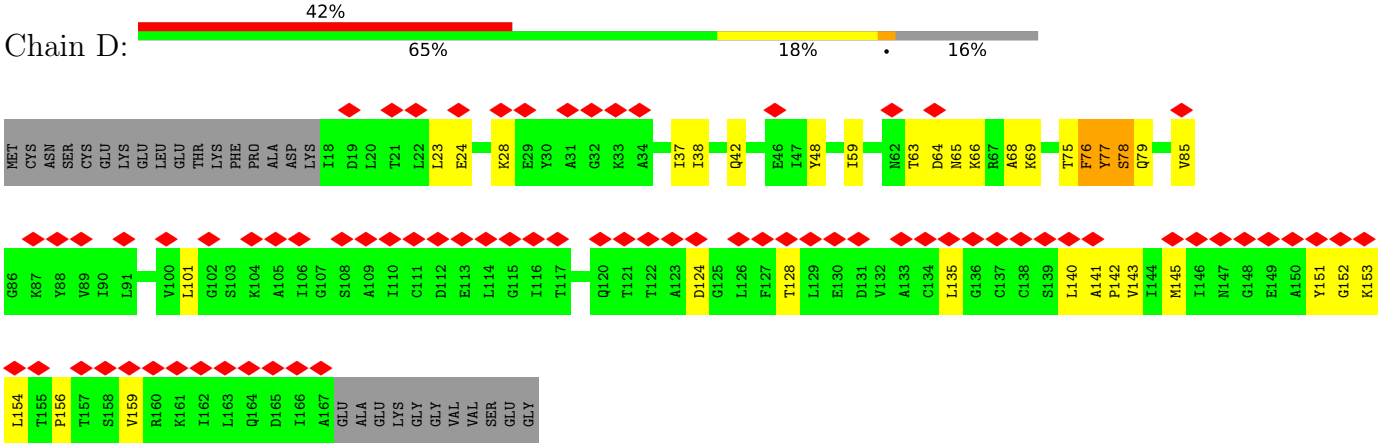
• Molecule 1: NAD-dependent formate dehydrogenase gamma subunit

Chain A:



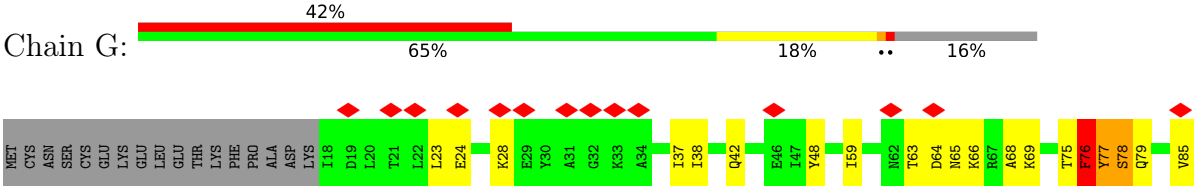
• Molecule 1: NAD-dependent formate dehydrogenase gamma subunit

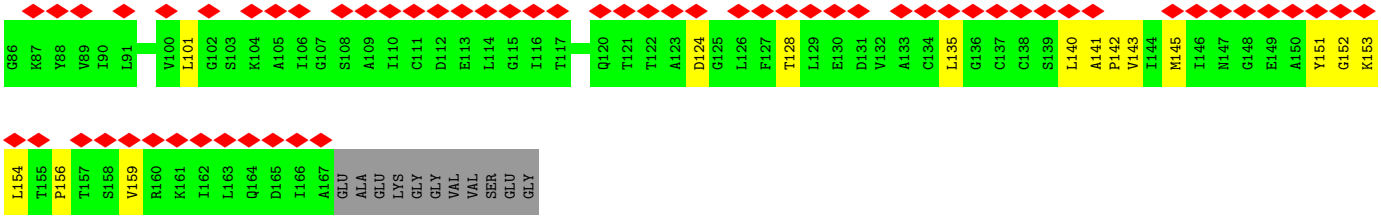
Chain D:



• Molecule 1: NAD-dependent formate dehydrogenase gamma subunit

Chain G:

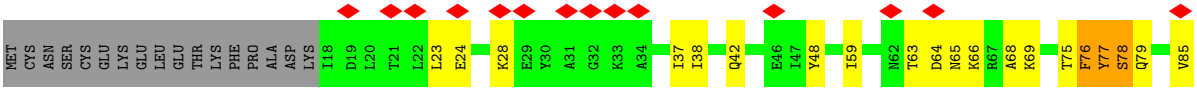


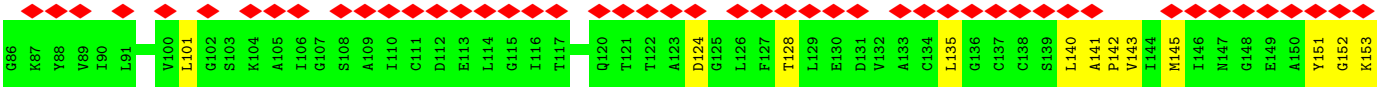


• Molecule 1: NAD-dependent formate dehydrogenase gamma subunit

Chain J:



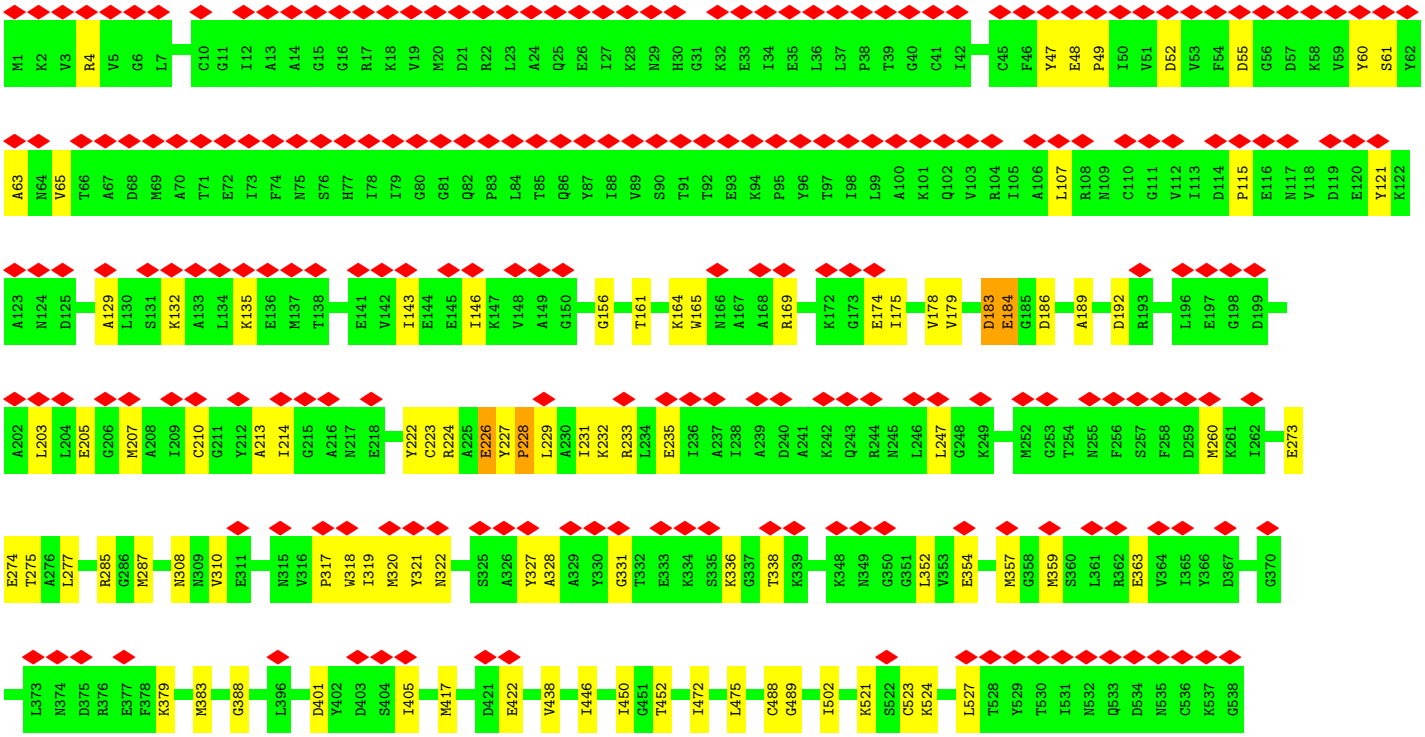


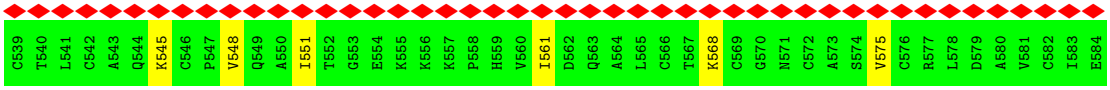


• Molecule 2: NAD-reducing hydrogenase subunit HoxF

Chain B:



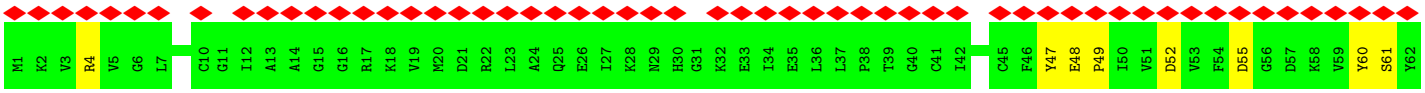


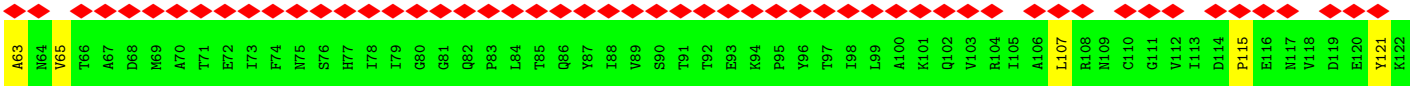


• Molecule 2: NAD-reducing hydrogenase subunit HoxF

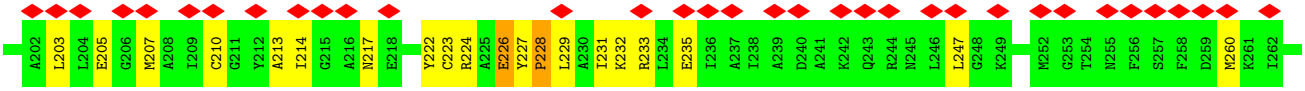
Chain E:

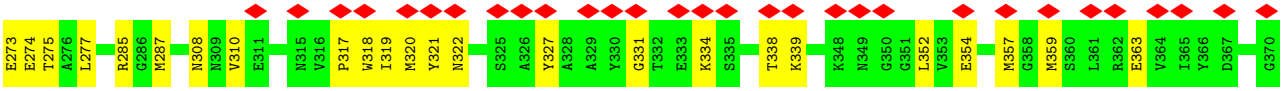


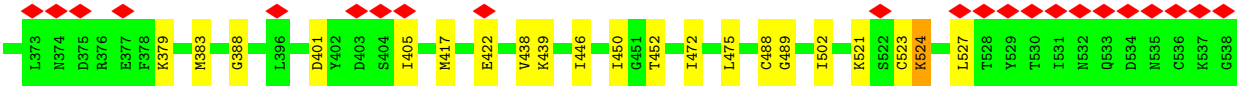


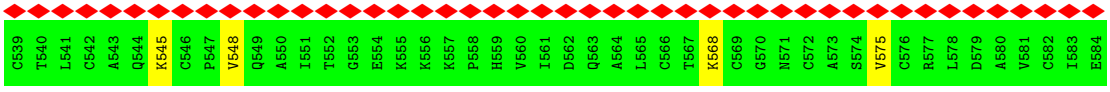








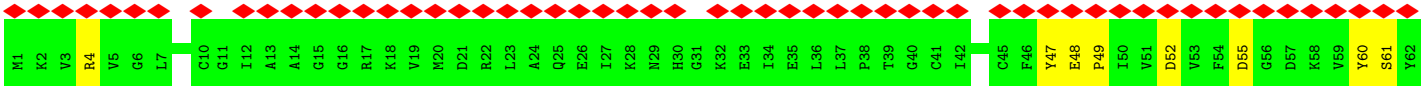


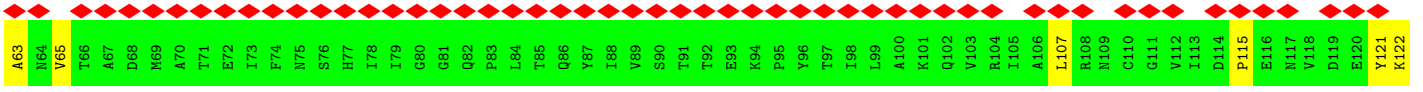


• Molecule 2: NAD-reducing hydrogenase subunit HoxF

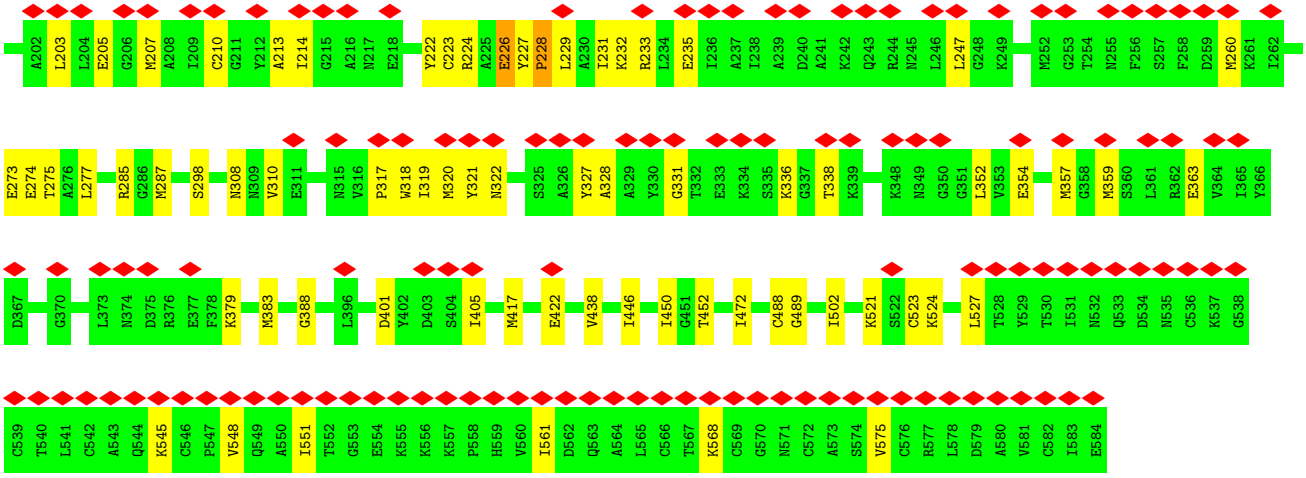
Chain H:







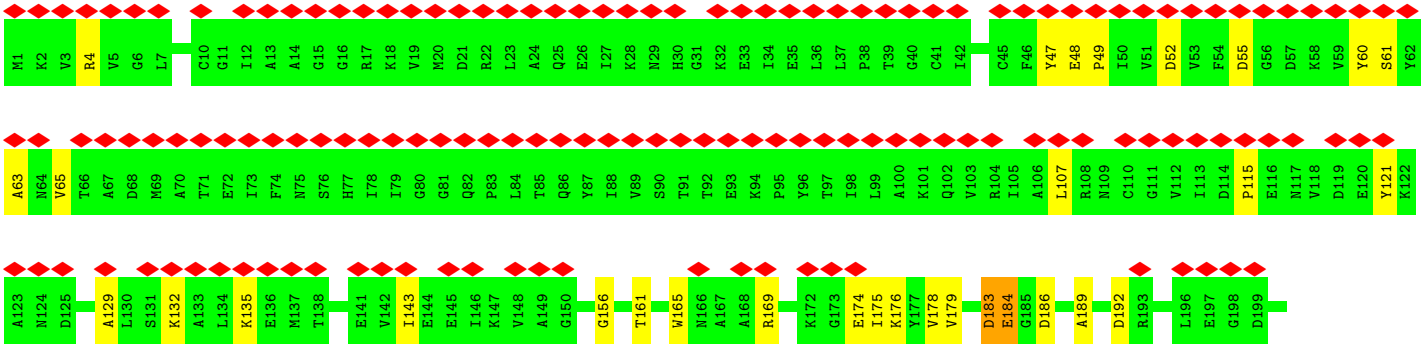




• Molecule 2: NAD-reducing hydrogenase subunit HoxF

Chain K:

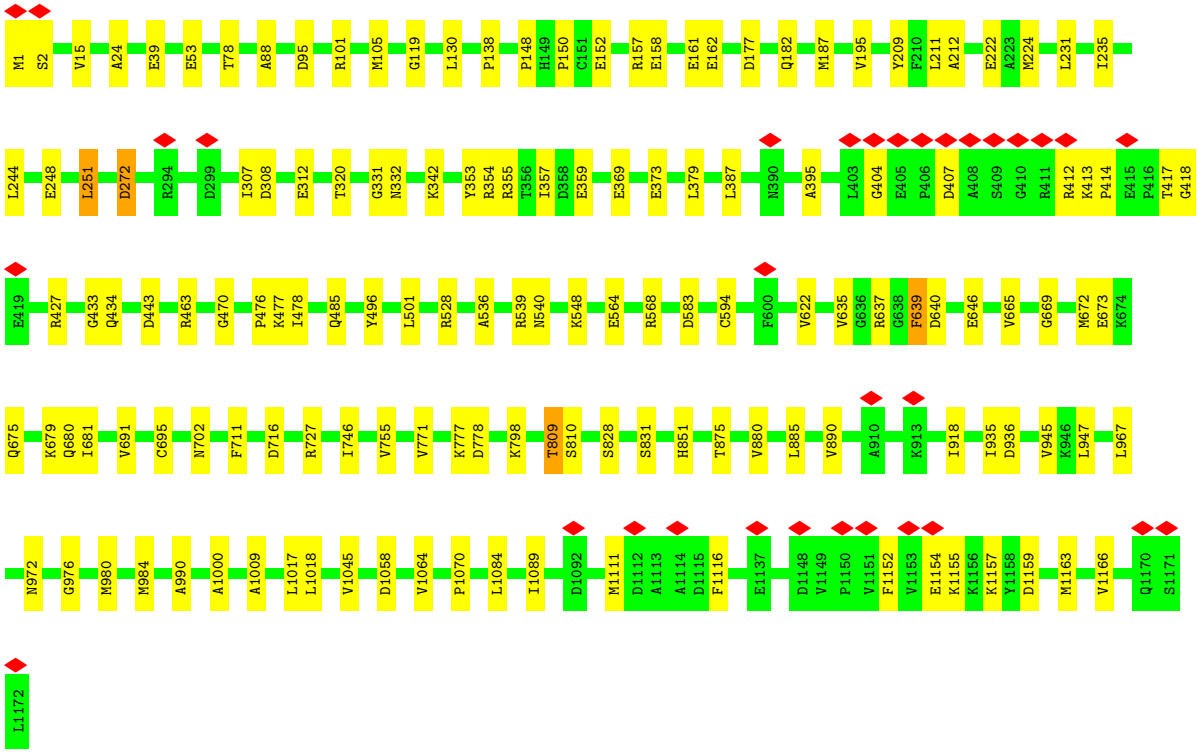




• Molecule 3: Formate dehydrogenase-O, major subunit

Chain C:

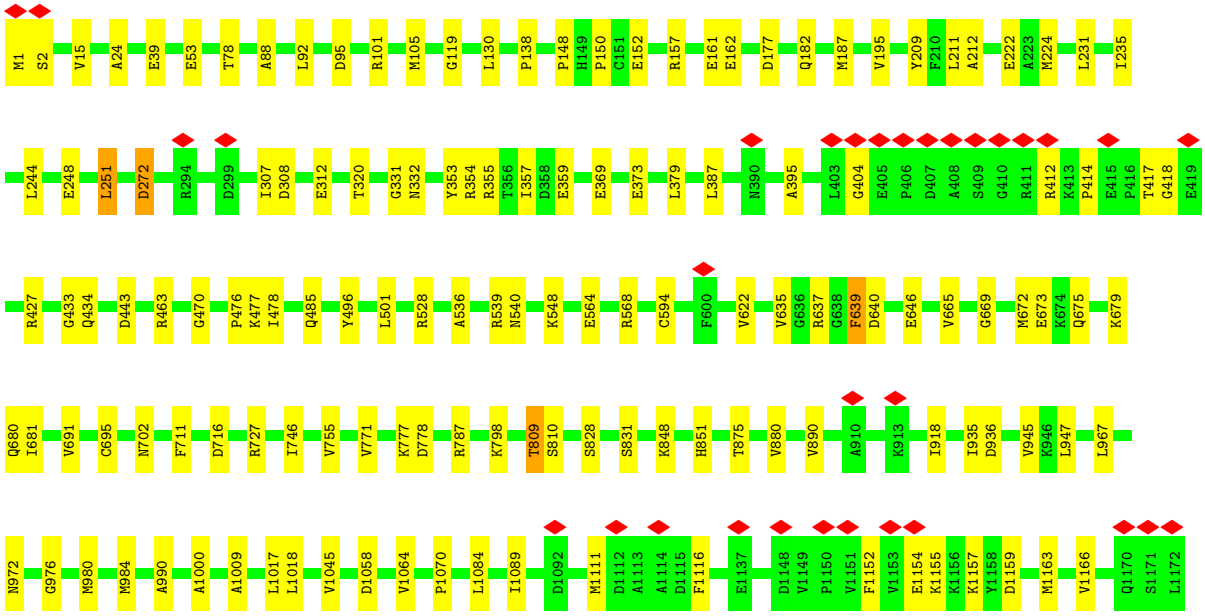




• Molecule 3: Formate dehydrogenase-O, major subunit

Chain F:

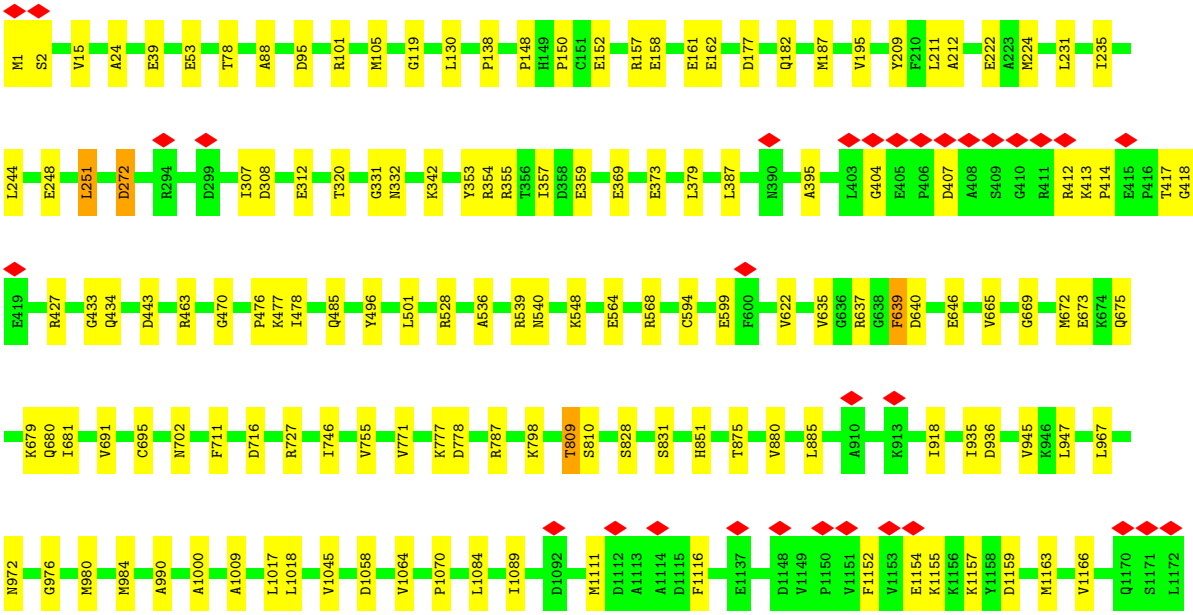




• Molecule 3: Formate dehydrogenase-O, major subunit

Chain I:

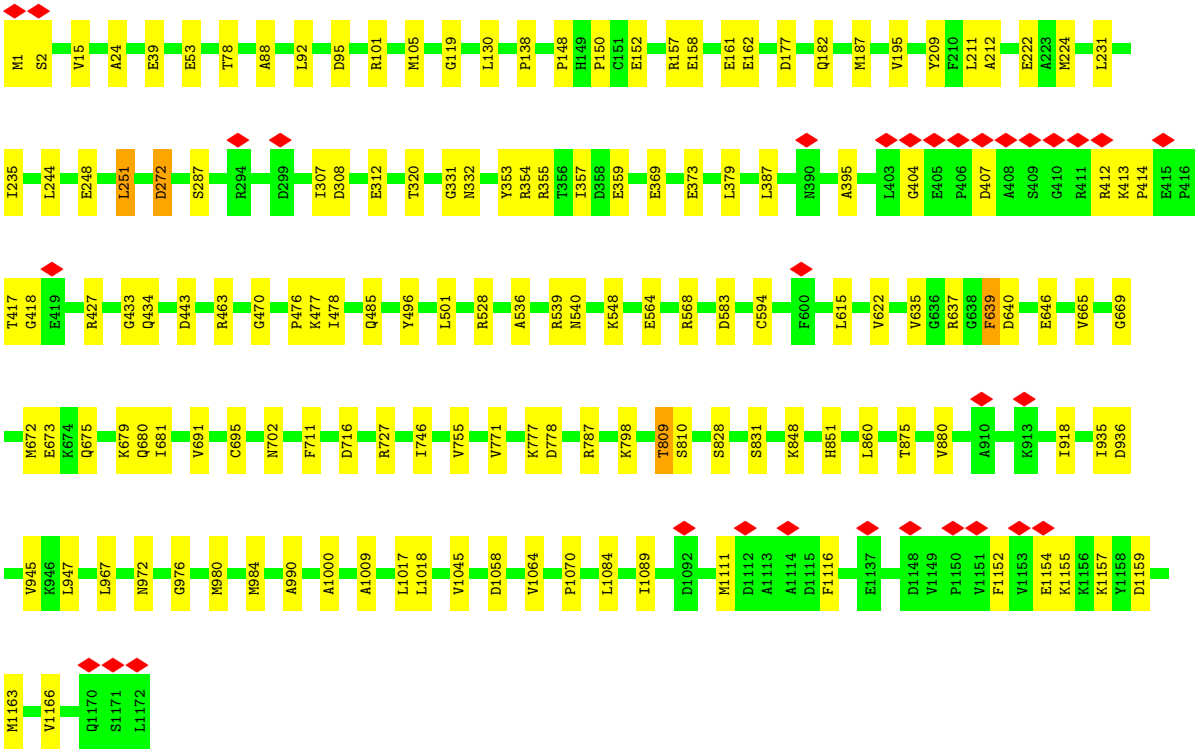




• Molecule 3: Formate dehydrogenase-O, major subunit

Chain L:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54596	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.749	Depositor
Minimum map value	-1.096	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.164	Depositor
Map size (Å)	340.0, 340.0, 340.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, FMN, NAD, ZN, NDP, SF4, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.18	0/1135	0.49	2/1540 (0.1%)
1	D	0.18	0/1135	0.50	2/1540 (0.1%)
1	G	0.18	0/1135	0.50	2/1540 (0.1%)
1	J	0.18	0/1135	0.50	2/1540 (0.1%)
2	B	0.23	0/4508	0.49	3/6074 (0.0%)
2	E	0.23	0/4508	0.49	3/6074 (0.0%)
2	H	0.23	0/4508	0.49	3/6074 (0.0%)
2	K	0.23	0/4508	0.49	3/6074 (0.0%)
3	C	0.23	0/8981	0.39	0/12161
3	F	0.23	0/8981	0.39	0/12161
3	I	0.23	0/8981	0.39	0/12161
3	L	0.23	0/8981	0.39	0/12161
All	All	0.23	0/58496	0.43	20/79100 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	E	0	1
2	H	0	1
2	K	0	1
All	All	0	4

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	226	GLU	N-CA-C	-7.12	104.96	112.93
2	B	226	GLU	N-CA-C	-7.11	104.97	112.93
2	E	226	GLU	N-CA-C	-7.08	105.00	112.93
2	H	226	GLU	N-CA-C	-7.06	105.02	112.93
1	D	76	PHE	CA-C-N	5.70	132.42	121.54
1	D	76	PHE	C-N-CA	5.70	132.42	121.54
1	A	76	PHE	CA-C-N	5.69	132.41	121.54
1	A	76	PHE	C-N-CA	5.69	132.41	121.54
1	G	76	PHE	CA-C-N	5.69	132.41	121.54
1	G	76	PHE	C-N-CA	5.69	132.41	121.54
1	J	76	PHE	CA-C-N	5.69	132.41	121.54
1	J	76	PHE	C-N-CA	5.69	132.41	121.54
2	E	523	CYS	CA-C-N	5.18	134.44	121.80
2	E	523	CYS	C-N-CA	5.18	134.44	121.80
2	B	523	CYS	CA-C-N	5.17	134.41	121.80
2	B	523	CYS	C-N-CA	5.17	134.41	121.80
2	H	523	CYS	CA-C-N	5.16	134.40	121.80
2	H	523	CYS	C-N-CA	5.16	134.40	121.80
2	K	523	CYS	CA-C-N	5.15	134.37	121.80
2	K	523	CYS	C-N-CA	5.15	134.37	121.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	224	ARG	Sidechain
2	E	224	ARG	Sidechain
2	H	224	ARG	Sidechain
2	K	224	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1118	0	1148	20	0
1	D	1118	0	1148	20	0
1	G	1118	0	1148	21	0
1	J	1118	0	1148	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4431	0	4443	65	0
2	E	4431	0	4443	68	0
2	H	4431	0	4443	65	0
2	K	4431	0	4443	68	0
3	C	8846	0	8905	94	0
3	F	8846	0	8905	93	0
3	I	8846	0	8905	96	0
3	L	8846	0	8905	97	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
4	G	4	0	0	0	0
4	H	4	0	0	0	0
4	I	4	0	0	0	0
4	J	4	0	0	0	0
4	K	4	0	0	0	0
4	L	4	0	0	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	H	1	0	0	0	0
5	K	1	0	0	0	0
6	B	31	0	19	3	0
6	E	31	0	19	4	0
6	H	31	0	19	3	0
6	K	31	0	19	5	0
7	B	24	0	0	2	0
7	C	48	0	0	1	0
7	E	24	0	0	2	0
7	F	48	0	0	1	0
7	H	24	0	0	2	0
7	I	48	0	0	1	0
7	K	24	0	0	2	0
7	L	48	0	0	1	0
8	B	44	0	26	3	0
8	E	44	0	26	3	0
8	H	44	0	26	3	0
8	K	44	0	26	3	0
9	C	53	0	31	0	0
9	F	53	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	53	0	31	0	0
9	L	53	0	31	1	0
10	C	48	0	26	6	0
10	F	48	0	26	6	0
10	I	48	0	26	6	0
10	L	48	0	26	6	0
All	All	58624	0	58392	714	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (714) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:GLU:HG3	2:B:192:ASP:HB2	1.45	0.97
2:K:184:GLU:HG3	2:K:192:ASP:HB2	1.45	0.97
2:E:184:GLU:HG3	2:E:192:ASP:HB2	1.45	0.97
2:H:184:GLU:HG3	2:H:192:ASP:HB2	1.45	0.97
1:J:154:LEU:HD21	1:J:159:VAL:HB	1.67	0.76
1:D:154:LEU:HD21	1:D:159:VAL:HB	1.67	0.75
1:G:154:LEU:HD21	1:G:159:VAL:HB	1.67	0.74
1:A:154:LEU:HD21	1:A:159:VAL:HB	1.67	0.73
2:B:156:GLY:HA3	8:B:606:NAD:H2N	1.73	0.71
2:H:156:GLY:HA3	8:H:606:NAD:H2N	1.73	0.71
2:B:285:ARG:HE	2:B:287:MET:HE3	1.56	0.71
2:H:285:ARG:HE	2:H:287:MET:HE3	1.56	0.71
3:F:332:ASN:ND2	10:F:1203:NDP:O7N	2.22	0.71
3:L:332:ASN:ND2	10:L:1203:NDP:O7N	2.22	0.71
2:K:156:GLY:HA3	8:K:606:NAD:H2N	1.73	0.71
2:E:156:GLY:HA3	8:E:606:NAD:H2N	1.73	0.71
2:E:285:ARG:HE	2:E:287:MET:HE3	1.56	0.69
2:K:285:ARG:HE	2:K:287:MET:HE3	1.56	0.69
2:B:227:TYR:O	2:B:231:ILE:HG12	1.93	0.69
2:H:227:TYR:O	2:H:231:ILE:HG12	1.93	0.69
2:E:227:TYR:O	2:E:231:ILE:HG12	1.93	0.68
2:K:227:TYR:O	2:K:231:ILE:HG12	1.93	0.68
2:B:174:GLU:HG2	2:B:175:ILE:HG13	1.74	0.68
2:H:174:GLU:HG2	2:H:175:ILE:HG13	1.74	0.68
3:L:331:GLY:HA3	10:L:1203:NDP:H1D	1.77	0.67
3:F:331:GLY:HA3	10:F:1203:NDP:H1D	1.77	0.67
3:L:244:LEU:O	3:L:248:GLU:HG3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:174:GLU:HG2	2:E:175:ILE:HG13	1.74	0.67
3:F:244:LEU:O	3:F:248:GLU:HG3	1.94	0.67
3:C:369:GLU:HG2	3:C:539:ARG:HH12	1.60	0.67
3:I:332:ASN:ND2	10:I:1203:NDP:O7N	2.22	0.67
2:K:174:GLU:HG2	2:K:175:ILE:HG13	1.74	0.67
2:B:260:MET:HA	2:B:260:MET:HE3	1.76	0.67
3:I:369:GLU:HG2	3:I:539:ARG:HH12	1.60	0.67
2:H:260:MET:HE3	2:H:260:MET:HA	1.76	0.66
3:I:331:GLY:HA3	10:I:1203:NDP:H1D	1.77	0.66
3:C:331:GLY:HA3	10:C:1203:NDP:H1D	1.77	0.66
3:C:332:ASN:ND2	10:C:1203:NDP:O7N	2.22	0.66
2:E:260:MET:HE3	2:E:260:MET:HA	1.76	0.66
3:C:244:LEU:O	3:C:248:GLU:HG3	1.94	0.66
2:K:260:MET:HE3	2:K:260:MET:HA	1.76	0.66
3:I:244:LEU:O	3:I:248:GLU:HG3	1.94	0.66
2:E:226:GLU:C	2:E:228:PRO:HD3	2.21	0.65
2:K:226:GLU:C	2:K:228:PRO:HD3	2.22	0.65
3:F:369:GLU:HG2	3:F:539:ARG:HH12	1.60	0.65
3:L:369:GLU:HG2	3:L:539:ARG:HH12	1.60	0.65
1:A:68:ALA:HB2	3:C:646:GLU:HG2	1.79	0.65
3:C:187:MET:HE3	3:C:212:ALA:O	1.97	0.65
3:I:187:MET:HE3	3:I:212:ALA:O	1.97	0.65
3:C:354:ARG:NH1	10:C:1203:NDP:O3X	2.30	0.65
3:F:152:GLU:OE1	3:F:528:ARG:NH2	2.30	0.65
1:G:68:ALA:HB2	3:I:646:GLU:HG2	1.79	0.65
3:L:152:GLU:OE1	3:L:528:ARG:NH2	2.30	0.65
1:D:68:ALA:HB2	3:F:646:GLU:HG2	1.79	0.65
3:I:354:ARG:NH1	10:I:1203:NDP:O3X	2.30	0.65
1:J:68:ALA:HB2	3:L:646:GLU:HG2	1.79	0.65
3:F:354:ARG:NH1	10:F:1203:NDP:O3X	2.30	0.64
3:L:354:ARG:NH1	10:L:1203:NDP:O3X	2.30	0.64
2:B:285:ARG:HE	2:B:287:MET:CE	2.10	0.64
2:H:226:GLU:C	2:H:228:PRO:HD3	2.21	0.64
2:H:285:ARG:HE	2:H:287:MET:CE	2.10	0.64
3:C:152:GLU:OE1	3:C:528:ARG:NH2	2.30	0.64
3:F:695:CYS:SG	3:F:727:ARG:NH2	2.71	0.64
3:I:152:GLU:OE1	3:I:528:ARG:NH2	2.30	0.64
2:K:285:ARG:HE	2:K:287:MET:CE	2.10	0.64
3:L:695:CYS:SG	3:L:727:ARG:NH2	2.71	0.64
2:B:226:GLU:C	2:B:228:PRO:HD3	2.22	0.64
2:E:285:ARG:HE	2:E:287:MET:CE	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:355:ARG:HD3	3:C:359:GLU:HG2	1.81	0.63
3:I:355:ARG:HD3	3:I:359:GLU:HG2	1.81	0.63
3:L:187:MET:HE3	3:L:212:ALA:O	1.97	0.63
3:L:355:ARG:HD3	3:L:359:GLU:HG2	1.80	0.63
3:F:187:MET:HE3	3:F:212:ALA:O	1.97	0.63
3:F:355:ARG:HD3	3:F:359:GLU:HG2	1.81	0.63
2:B:107:LEU:HD11	2:B:352:LEU:HD22	1.81	0.62
3:C:695:CYS:SG	3:C:727:ARG:NH2	2.71	0.62
2:H:107:LEU:HD11	2:H:352:LEU:HD22	1.81	0.62
2:K:107:LEU:HD11	2:K:352:LEU:HD22	1.81	0.62
2:E:107:LEU:HD11	2:E:352:LEU:HD22	1.81	0.62
3:I:695:CYS:SG	3:I:727:ARG:NH2	2.71	0.62
2:B:357:MET:N	2:B:357:MET:SD	2.67	0.62
2:H:357:MET:SD	2:H:357:MET:N	2.67	0.61
3:F:477:LYS:O	10:F:1203:NDP:N7N	2.34	0.61
3:L:477:LYS:O	10:L:1203:NDP:N7N	2.34	0.61
1:A:77:TYR:O	1:A:79:GLN:N	2.34	0.60
1:G:77:TYR:O	1:G:79:GLN:N	2.34	0.60
3:C:477:LYS:O	10:C:1203:NDP:N7N	2.34	0.60
1:J:77:TYR:O	1:J:79:GLN:N	2.34	0.60
1:D:77:TYR:O	1:D:79:GLN:N	2.34	0.60
3:F:470:GLY:N	3:F:485:GLN:OE1	2.33	0.60
3:I:477:LYS:O	10:I:1203:NDP:N7N	2.34	0.60
3:L:470:GLY:N	3:L:485:GLN:OE1	2.33	0.60
3:C:496:TYR:HB2	3:C:501:LEU:HD13	1.84	0.59
3:I:496:TYR:HB2	3:I:501:LEU:HD13	1.84	0.59
3:F:880:VAL:HG12	3:F:918:ILE:HG21	1.83	0.59
3:I:880:VAL:HG12	3:I:918:ILE:HG21	1.83	0.59
2:K:331:GLY:HA3	2:K:357:MET:SD	2.43	0.59
3:L:880:VAL:HG12	3:L:918:ILE:HG21	1.83	0.59
3:C:880:VAL:HG12	3:C:918:ILE:HG21	1.83	0.59
2:E:331:GLY:HA3	2:E:357:MET:SD	2.43	0.59
3:F:222:GLU:HG3	3:F:224:MET:H	1.66	0.59
3:L:222:GLU:HG3	3:L:224:MET:H	1.66	0.59
2:B:331:GLY:HA3	2:B:357:MET:SD	2.43	0.59
2:H:331:GLY:HA3	2:H:357:MET:SD	2.43	0.59
3:C:222:GLU:HG3	3:C:224:MET:H	1.66	0.59
2:E:228:PRO:O	2:E:229:LEU:C	2.46	0.59
1:D:38:ILE:O	1:D:42:GLN:HG3	2.03	0.58
1:J:38:ILE:O	1:J:42:GLN:HG3	2.03	0.58
2:K:228:PRO:O	2:K:229:LEU:C	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:222:GLU:HG3	3:I:224:MET:H	1.66	0.58
3:F:496:TYR:HB2	3:F:501:LEU:HD13	1.84	0.58
3:L:496:TYR:HB2	3:L:501:LEU:HD13	1.84	0.58
1:A:38:ILE:O	1:A:42:GLN:HG3	2.03	0.58
1:G:38:ILE:O	1:G:42:GLN:HG3	2.03	0.58
2:H:132:LYS:NZ	2:H:321:TYR:O	2.34	0.58
2:B:132:LYS:NZ	2:B:321:TYR:O	2.34	0.58
2:E:228:PRO:O	2:E:231:ILE:N	2.37	0.58
2:E:357:MET:SD	2:E:357:MET:N	2.67	0.58
2:K:228:PRO:O	2:K:231:ILE:N	2.37	0.58
2:B:450:ILE:HA	3:C:639:PHE:HE2	1.68	0.58
2:H:450:ILE:HA	3:I:639:PHE:HE2	1.69	0.58
3:C:470:GLY:N	3:C:485:GLN:OE1	2.33	0.57
3:I:777:LYS:NZ	3:I:778:ASP:OD2	2.37	0.57
3:C:777:LYS:NZ	3:C:778:ASP:OD2	2.37	0.57
2:E:472:ILE:HG23	2:E:502:ILE:HD11	1.85	0.57
2:H:472:ILE:HG23	2:H:502:ILE:HD11	1.85	0.57
3:I:470:GLY:N	3:I:485:GLN:OE1	2.33	0.57
2:K:203:LEU:HD13	2:K:310:VAL:HG13	1.85	0.57
2:K:357:MET:SD	2:K:357:MET:N	2.67	0.57
2:K:472:ILE:HG23	2:K:502:ILE:HD11	1.85	0.57
2:B:472:ILE:HG23	2:B:502:ILE:HD11	1.85	0.57
2:E:203:LEU:HD13	2:E:310:VAL:HG13	1.85	0.57
3:F:777:LYS:NZ	3:F:778:ASP:OD2	2.37	0.57
2:H:203:LEU:HD13	2:H:310:VAL:HG13	1.85	0.57
2:B:228:PRO:O	2:B:229:LEU:C	2.46	0.57
3:L:777:LYS:NZ	3:L:778:ASP:OD2	2.37	0.57
2:B:183:ASP:OD2	2:B:183:ASP:N	2.37	0.57
2:B:203:LEU:HD13	2:B:310:VAL:HG13	1.85	0.57
2:H:228:PRO:O	2:H:231:ILE:N	2.37	0.57
2:H:183:ASP:OD2	2:H:183:ASP:N	2.37	0.57
2:B:228:PRO:O	2:B:231:ILE:N	2.37	0.57
2:E:48:GLU:HG3	2:E:49:PRO:HA	1.87	0.57
2:H:228:PRO:O	2:H:229:LEU:C	2.46	0.57
2:K:48:GLU:HG3	2:K:49:PRO:HA	1.87	0.57
2:K:132:LYS:NZ	2:K:321:TYR:O	2.34	0.56
2:K:273:GLU:OE1	2:K:275:THR:OG1	2.23	0.56
2:B:273:GLU:OE1	2:B:275:THR:OG1	2.23	0.56
2:E:132:LYS:NZ	2:E:321:TYR:O	2.34	0.56
2:E:161:THR:O	2:E:165:TRP:N	2.32	0.56
2:E:183:ASP:OD2	2:E:183:ASP:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:273:GLU:OE1	2:E:275:THR:OG1	2.23	0.56
2:H:273:GLU:OE1	2:H:275:THR:OG1	2.23	0.56
3:F:308:ASP:O	3:F:312:GLU:HG3	2.06	0.56
2:K:161:THR:O	2:K:165:TRP:N	2.32	0.56
2:K:183:ASP:N	2:K:183:ASP:OD2	2.37	0.56
3:L:308:ASP:O	3:L:312:GLU:HG3	2.06	0.56
3:F:1045:VAL:HG11	3:F:1070:PRO:HB3	1.88	0.56
3:C:404:GLY:O	3:C:412:ARG:NE	2.38	0.56
2:E:450:ILE:HA	3:F:639:PHE:HE2	1.68	0.56
2:K:450:ILE:HA	3:L:639:PHE:HE2	1.68	0.56
3:L:1045:VAL:HG11	3:L:1070:PRO:HB3	1.88	0.56
3:I:404:GLY:O	3:I:412:ARG:NE	2.38	0.56
2:K:183:ASP:OD2	2:K:222:TYR:HD1	1.88	0.56
2:B:183:ASP:OD2	2:B:222:TYR:HD1	1.88	0.56
2:E:183:ASP:OD2	2:E:222:TYR:HD1	1.88	0.56
3:C:1045:VAL:HG11	3:C:1070:PRO:HB3	1.88	0.55
2:H:183:ASP:OD2	2:H:222:TYR:HD1	1.88	0.55
3:L:976:GLY:O	3:L:980:MET:HG2	2.06	0.55
3:C:308:ASP:O	3:C:312:GLU:HG3	2.06	0.55
3:F:976:GLY:O	3:F:980:MET:HG2	2.06	0.55
3:I:308:ASP:O	3:I:312:GLU:HG3	2.06	0.55
3:I:1045:VAL:HG11	3:I:1070:PRO:HB3	1.88	0.55
3:C:976:GLY:O	3:C:980:MET:HG2	2.06	0.55
3:I:976:GLY:O	3:I:980:MET:HG2	2.06	0.55
3:F:404:GLY:O	3:F:412:ARG:NE	2.38	0.55
2:H:48:GLU:HG3	2:H:49:PRO:HA	1.87	0.55
1:D:59:ILE:O	1:D:63:THR:OG1	2.25	0.55
3:L:404:GLY:O	3:L:412:ARG:NE	2.38	0.55
2:B:48:GLU:HG3	2:B:49:PRO:HA	1.87	0.55
1:J:59:ILE:O	1:J:63:THR:OG1	2.25	0.55
2:K:320:MET:HA	2:K:320:MET:HE2	1.90	0.55
2:B:161:THR:O	2:B:165:TRP:N	2.32	0.54
3:C:568:ARG:NH2	3:C:673:GLU:O	2.40	0.54
2:E:320:MET:HE2	2:E:320:MET:HA	1.90	0.54
1:G:59:ILE:O	1:G:63:THR:OG1	2.25	0.54
2:H:161:THR:O	2:H:165:TRP:N	2.32	0.54
1:A:59:ILE:O	1:A:63:THR:OG1	2.25	0.54
3:I:568:ARG:NH2	3:I:673:GLU:O	2.40	0.54
3:C:809:THR:OG1	3:C:810:SER:N	2.40	0.54
3:I:809:THR:OG1	3:I:810:SER:N	2.40	0.54
2:K:308:ASN:ND2	6:K:603:FMN:O1P	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:434:GLN:HB2	3:L:476:PRO:HG3	1.90	0.54
2:B:179:VAL:HG11	2:B:277:LEU:HD21	1.90	0.54
2:E:308:ASN:ND2	6:E:603:FMN:O1P	2.41	0.54
3:F:434:GLN:HB2	3:F:476:PRO:HG3	1.90	0.54
3:F:809:THR:OG1	3:F:810:SER:N	2.40	0.54
2:B:320:MET:HE2	2:B:320:MET:HA	1.90	0.53
2:H:179:VAL:HG11	2:H:277:LEU:HD21	1.90	0.53
2:H:320:MET:HE2	2:H:320:MET:HA	1.90	0.53
3:L:809:THR:OG1	3:L:810:SER:N	2.40	0.53
3:L:568:ARG:NH2	3:L:673:GLU:O	2.40	0.53
3:C:434:GLN:HB2	3:C:476:PRO:HG3	1.90	0.53
2:E:274:GLU:OE2	8:E:606:NAD:O2B	2.23	0.53
3:F:568:ARG:NH2	3:F:673:GLU:O	2.40	0.53
2:H:308:ASN:ND2	6:H:603:FMN:O1P	2.41	0.53
3:I:434:GLN:HB2	3:I:476:PRO:HG3	1.90	0.53
2:K:274:GLU:OE2	8:K:606:NAD:O2B	2.23	0.53
2:B:308:ASN:ND2	6:B:603:FMN:O1P	2.41	0.53
2:K:383:MET:O	2:K:388:GLY:HA3	2.09	0.53
2:E:383:MET:O	2:E:388:GLY:HA3	2.09	0.53
1:A:78:SER:HB3	3:C:637:ARG:HH12	1.74	0.52
2:K:179:VAL:HG11	2:K:277:LEU:HD21	1.90	0.52
1:D:78:SER:HB3	3:F:637:ARG:HH12	1.74	0.52
2:E:179:VAL:HG11	2:E:277:LEU:HD21	1.90	0.52
1:G:78:SER:HB3	3:I:637:ARG:HH12	1.74	0.52
3:I:1:MET:HG2	3:I:2:SER:H	1.75	0.52
3:C:1:MET:HG2	3:C:2:SER:H	1.75	0.52
1:J:78:SER:HB3	3:L:637:ARG:HH12	1.74	0.52
2:B:383:MET:O	2:B:388:GLY:HA3	2.09	0.52
2:E:169:ARG:NH1	2:E:213:ALA:O	2.43	0.52
2:H:383:MET:O	2:H:388:GLY:HA3	2.09	0.52
2:K:169:ARG:NH1	2:K:213:ALA:O	2.43	0.52
6:H:603:FMN:O2'	8:H:606:NAD:O2N	2.27	0.52
6:B:603:FMN:O2'	8:B:606:NAD:O2N	2.27	0.52
3:F:990:ALA:HA	3:F:1017:LEU:HD21	1.92	0.52
3:L:990:ALA:HA	3:L:1017:LEU:HD21	1.92	0.52
2:B:169:ARG:NH1	2:B:213:ALA:O	2.43	0.52
2:H:169:ARG:NH1	2:H:213:ALA:O	2.43	0.51
2:B:52:ASP:OD1	2:B:61:SER:OG	2.23	0.51
3:L:702:ASN:ND2	3:L:716:ASP:OD1	2.42	0.51
3:L:972:ASN:N	3:L:972:ASN:OD1	2.42	0.51
3:F:669:GLY:O	3:F:672:MET:HE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:702:ASN:ND2	3:F:716:ASP:OD1	2.42	0.51
3:F:972:ASN:OD1	3:F:972:ASN:N	2.42	0.51
3:L:669:GLY:O	3:L:672:MET:HE2	2.10	0.51
2:H:52:ASP:OD1	2:H:61:SER:OG	2.23	0.51
3:C:990:ALA:HA	3:C:1017:LEU:HD21	1.92	0.51
3:I:990:ALA:HA	3:I:1017:LEU:HD21	1.92	0.51
3:L:1:MET:HG2	3:L:2:SER:H	1.75	0.51
6:E:603:FMN:O2'	8:E:606:NAD:O2N	2.27	0.51
3:F:1:MET:HG2	3:F:2:SER:H	1.75	0.50
3:C:669:GLY:O	3:C:672:MET:HE2	2.11	0.50
1:G:124:ASP:OD1	1:G:124:ASP:N	2.44	0.50
1:A:124:ASP:OD1	1:A:124:ASP:N	2.44	0.50
2:B:318:TRP:O	2:B:327:TYR:OH	2.19	0.50
3:C:702:ASN:ND2	3:C:716:ASP:OD1	2.42	0.50
3:I:669:GLY:O	3:I:672:MET:HE2	2.11	0.50
3:I:702:ASN:ND2	3:I:716:ASP:OD1	2.42	0.50
6:K:603:FMN:O2'	8:K:606:NAD:O2N	2.27	0.50
3:C:564:GLU:OE2	3:C:679:LYS:NZ	2.35	0.50
3:C:828:SER:HB3	3:C:967:LEU:H	1.77	0.50
3:L:828:SER:HB3	3:L:967:LEU:H	1.77	0.50
2:E:568:LYS:N	7:E:604:SF4:S2	2.85	0.50
3:F:828:SER:HB3	3:F:967:LEU:H	1.77	0.50
3:I:828:SER:HB3	3:I:967:LEU:H	1.77	0.50
2:K:568:LYS:N	7:K:604:SF4:S2	2.85	0.50
2:B:568:LYS:N	7:B:604:SF4:S2	2.85	0.50
2:H:318:TRP:O	2:H:327:TYR:OH	2.19	0.50
2:H:568:LYS:N	7:H:604:SF4:S2	2.85	0.50
3:I:138:PRO:HB3	3:I:209:TYR:CG	2.47	0.50
3:C:138:PRO:HB3	3:C:209:TYR:CG	2.47	0.49
2:E:318:TRP:O	2:E:327:TYR:OH	2.19	0.49
2:E:338:THR:OG1	2:E:354:GLU:OE2	2.26	0.49
2:E:359:MET:HE3	2:E:363:GLU:HB3	1.93	0.49
2:H:338:THR:OG1	2:H:354:GLU:OE2	2.26	0.49
2:K:318:TRP:O	2:K:327:TYR:OH	2.19	0.49
2:K:338:THR:OG1	2:K:354:GLU:OE2	2.26	0.49
2:K:359:MET:HE3	2:K:363:GLU:HB3	1.93	0.49
1:A:76:PHE:O	1:A:78:SER:N	2.40	0.49
3:C:972:ASN:OD1	3:C:972:ASN:N	2.42	0.49
3:I:231:LEU:HA	3:I:235:ILE:HG13	1.94	0.49
3:L:138:PRO:HB3	3:L:209:TYR:CG	2.47	0.49
3:L:1152:PHE:HZ	3:L:1155:LYS:HG3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:PRO:HD2	7:C:1206:SF4:S4	2.53	0.49
3:C:231:LEU:HA	3:C:235:ILE:HG13	1.94	0.49
3:F:138:PRO:HB3	3:F:209:TYR:CG	2.47	0.49
3:F:1152:PHE:HZ	3:F:1155:LYS:HG3	1.78	0.49
3:I:150:PRO:HD2	7:I:1206:SF4:S4	2.53	0.49
2:K:178:VAL:HG22	2:K:214:ILE:HD11	1.94	0.49
1:G:76:PHE:O	1:G:78:SER:N	2.40	0.49
3:I:972:ASN:OD1	3:I:972:ASN:N	2.42	0.49
1:A:140:LEU:HB3	1:A:152:GLY:HA3	1.95	0.49
2:B:359:MET:HE3	2:B:363:GLU:HB3	1.93	0.49
2:E:178:VAL:HG22	2:E:214:ILE:HD11	1.94	0.49
2:H:359:MET:HE3	2:H:363:GLU:HB3	1.93	0.49
3:F:691:VAL:HG22	3:F:1064:VAL:HG22	1.95	0.49
1:G:140:LEU:HB3	1:G:152:GLY:HA3	1.95	0.49
3:L:691:VAL:HG22	3:L:1064:VAL:HG22	1.95	0.49
3:F:357:ILE:HG13	3:F:379:LEU:HD11	1.94	0.49
2:K:63:ALA:HA	2:K:65:VAL:HG23	1.94	0.48
3:L:231:LEU:HA	3:L:235:ILE:HG13	1.94	0.48
2:B:446:ILE:HD11	3:C:88:ALA:HB1	1.96	0.48
3:F:231:LEU:HA	3:F:235:ILE:HG13	1.94	0.48
2:H:446:ILE:HD11	3:I:88:ALA:HB1	1.96	0.48
3:L:150:PRO:HD2	7:L:1206:SF4:S4	2.53	0.48
3:L:357:ILE:HG13	3:L:379:LEU:HD11	1.94	0.48
2:E:63:ALA:HA	2:E:65:VAL:HG23	1.95	0.48
3:F:150:PRO:HD2	7:F:1206:SF4:S4	2.53	0.48
3:I:564:GLU:OE2	3:I:679:LYS:NZ	2.35	0.48
3:C:357:ILE:HG13	3:C:379:LEU:HD11	1.94	0.48
3:I:357:ILE:HG13	3:I:379:LEU:HD11	1.94	0.48
2:B:178:VAL:HG22	2:B:214:ILE:HD11	1.94	0.48
3:C:622:VAL:HG21	3:C:665:VAL:HG11	1.95	0.48
3:C:1084:LEU:HD22	3:C:1089:ILE:HD12	1.95	0.48
2:E:164:LYS:HE3	2:E:164:LYS:HB3	1.72	0.48
3:F:622:VAL:HG21	3:F:665:VAL:HG11	1.95	0.48
2:H:178:VAL:HG22	2:H:214:ILE:HD11	1.94	0.48
3:L:622:VAL:HG21	3:L:665:VAL:HG11	1.95	0.48
3:L:1084:LEU:HD22	3:L:1089:ILE:HD12	1.95	0.48
2:B:274:GLU:OE2	8:B:606:NAD:O2B	2.23	0.48
3:C:433:GLY:HA2	10:C:1203:NDP:H4D	1.96	0.48
2:E:446:ILE:HD11	3:F:88:ALA:HB1	1.96	0.48
3:F:1084:LEU:HD22	3:F:1089:ILE:HD12	1.95	0.48
2:H:274:GLU:OE2	8:H:606:NAD:O2B	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:322:ASN:ND2	2:H:327:TYR:OH	2.31	0.48
3:I:622:VAL:HG21	3:I:665:VAL:HG11	1.95	0.48
2:K:446:ILE:HD11	3:L:88:ALA:HB1	1.96	0.48
2:B:63:ALA:HA	2:B:65:VAL:HG23	1.95	0.48
3:C:320:THR:HG23	3:C:427:ARG:CZ	2.44	0.48
2:H:63:ALA:HA	2:H:65:VAL:HG23	1.95	0.48
3:I:320:THR:HG23	3:I:427:ARG:CZ	2.44	0.48
3:I:433:GLY:HA2	10:I:1203:NDP:H4D	1.96	0.48
3:I:1152:PHE:HZ	3:I:1155:LYS:HG3	1.78	0.48
3:C:1152:PHE:HZ	3:C:1155:LYS:HG3	1.78	0.47
3:I:1084:LEU:HD22	3:I:1089:ILE:HD12	1.95	0.47
3:L:1157:LYS:HE3	3:L:1166:VAL:HG21	1.96	0.47
2:B:322:ASN:ND2	2:B:327:TYR:OH	2.31	0.47
3:F:1157:LYS:HE3	3:F:1166:VAL:HG21	1.96	0.47
3:I:691:VAL:HG22	3:I:1064:VAL:HG22	1.95	0.47
3:C:691:VAL:HG22	3:C:1064:VAL:HG22	1.95	0.47
3:L:320:THR:HG23	3:L:427:ARG:CZ	2.44	0.47
3:F:320:THR:HG23	3:F:427:ARG:CZ	2.44	0.47
3:F:851:HIS:NE2	3:F:936:ASP:OD1	2.46	0.47
1:J:140:LEU:HB3	1:J:152:GLY:HA3	1.95	0.47
3:L:851:HIS:NE2	3:L:936:ASP:OD1	2.46	0.47
3:L:355:ARG:HE	3:L:414:PRO:HD3	1.78	0.47
3:F:355:ARG:HE	3:F:414:PRO:HD3	1.78	0.47
3:C:272:ASP:OD2	3:C:272:ASP:N	2.48	0.47
1:D:140:LEU:HB3	1:D:152:GLY:HA3	1.95	0.47
2:E:379:LYS:HD2	2:E:422:GLU:HA	1.97	0.47
3:F:130:LEU:HD22	3:F:177:ASP:HB2	1.97	0.47
3:I:272:ASP:OD2	3:I:272:ASP:N	2.48	0.47
2:K:379:LYS:HD2	2:K:422:GLU:HA	1.97	0.47
1:A:85:VAL:HG12	1:A:128:THR:HG21	1.97	0.47
2:B:338:THR:OG1	2:B:354:GLU:OE2	2.26	0.47
1:J:85:VAL:HG12	1:J:128:THR:HG21	1.97	0.47
3:L:130:LEU:HD22	3:L:177:ASP:HB2	1.97	0.47
1:D:85:VAL:HG12	1:D:128:THR:HG21	1.97	0.46
2:E:52:ASP:OD1	2:E:61:SER:OG	2.23	0.46
3:F:162:GLU:HG3	3:F:528:ARG:HB2	1.97	0.46
1:G:85:VAL:HG12	1:G:128:THR:HG21	1.97	0.46
3:I:1:MET:HG2	3:I:2:SER:N	2.30	0.46
3:I:1157:LYS:HE3	3:I:1166:VAL:HG21	1.96	0.46
3:C:355:ARG:HE	3:C:414:PRO:HD3	1.78	0.46
3:L:162:GLU:HG3	3:L:528:ARG:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:MET:HG2	3:C:2:SER:N	2.30	0.46
3:C:1157:LYS:HE3	3:C:1166:VAL:HG21	1.96	0.46
2:E:401:ASP:O	2:E:405:ILE:HG12	2.16	0.46
3:I:119:GLY:HA3	3:I:681:ILE:HG21	1.97	0.46
3:I:417:THR:OG1	3:I:418:GLY:N	2.48	0.46
2:K:52:ASP:OD1	2:K:61:SER:OG	2.23	0.46
2:K:401:ASP:O	2:K:405:ILE:HG12	2.16	0.46
3:C:119:GLY:HA3	3:C:681:ILE:HG21	1.97	0.46
3:C:417:THR:OG1	3:C:418:GLY:N	2.48	0.46
6:B:603:FMN:O2'	6:B:603:FMN:O4'	2.32	0.46
6:H:603:FMN:O2'	6:H:603:FMN:O4'	2.32	0.46
3:L:417:THR:OG1	3:L:418:GLY:N	2.48	0.46
3:C:162:GLU:HG3	3:C:528:ARG:HB2	1.97	0.46
3:C:1009:ALA:HB2	3:C:1018:LEU:HD12	1.97	0.46
3:F:119:GLY:HA3	3:F:681:ILE:HG21	1.97	0.46
3:F:417:THR:OG1	3:F:418:GLY:N	2.48	0.46
2:H:488:CYS:SG	2:H:489:GLY:N	2.89	0.46
3:I:162:GLU:HG3	3:I:528:ARG:HB2	1.97	0.46
3:I:355:ARG:HE	3:I:414:PRO:HD3	1.78	0.46
2:K:169:ARG:O	2:K:176:LYS:NZ	2.40	0.46
3:L:119:GLY:HA3	3:L:681:ILE:HG21	1.97	0.46
2:E:169:ARG:O	2:E:176:LYS:NZ	2.40	0.46
3:F:433:GLY:HA2	10:F:1203:NDP:H4D	1.96	0.46
3:I:1009:ALA:HB2	3:I:1018:LEU:HD12	1.97	0.46
3:I:809:THR:HB	3:I:984:MET:HB3	1.98	0.46
3:C:771:VAL:HG21	3:C:1000:ALA:HB2	1.98	0.46
3:C:809:THR:HB	3:C:984:MET:HB3	1.98	0.46
3:C:1111:MET:HG3	3:C:1116:PHE:HZ	1.81	0.46
2:E:488:CYS:SG	2:E:489:GLY:N	2.88	0.46
3:I:1111:MET:HG3	3:I:1116:PHE:HZ	1.81	0.46
3:L:433:GLY:HA2	10:L:1203:NDP:H4D	1.96	0.46
2:B:401:ASP:O	2:B:405:ILE:HG12	2.16	0.46
2:B:488:CYS:SG	2:B:489:GLY:N	2.89	0.46
3:I:771:VAL:HG21	3:I:1000:ALA:HB2	1.98	0.46
2:K:488:CYS:SG	2:K:489:GLY:N	2.88	0.46
3:F:1:MET:HG2	3:F:2:SER:N	2.30	0.45
3:F:548:LYS:HE2	3:F:548:LYS:HB3	1.84	0.45
2:H:401:ASP:O	2:H:405:ILE:HG12	2.16	0.45
3:L:1:MET:HG2	3:L:2:SER:N	2.30	0.45
3:F:272:ASP:OD2	3:F:272:ASP:N	2.48	0.45
3:F:809:THR:HB	3:F:984:MET:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:135:LYS:HD3	2:K:135:LYS:HA	1.80	0.45
3:L:809:THR:HB	3:L:984:MET:HB3	1.98	0.45
2:B:207:MET:HA	2:B:210:CYS:SG	2.57	0.45
3:C:130:LEU:HD22	3:C:177:ASP:HB2	1.97	0.45
3:F:771:VAL:HG21	3:F:1000:ALA:HB2	1.98	0.45
1:G:24:GLU:O	1:G:28:LYS:HB3	2.17	0.45
2:H:247:LEU:HD11	2:H:260:MET:HG2	1.99	0.45
2:H:379:LYS:HD2	2:H:422:GLU:HA	1.97	0.45
3:I:599:GLU:H	3:I:599:GLU:HG3	1.60	0.45
3:L:272:ASP:N	3:L:272:ASP:OD2	2.48	0.45
1:A:24:GLU:O	1:A:28:LYS:HB3	2.17	0.45
2:B:247:LEU:HD11	2:B:260:MET:HG2	1.99	0.45
2:B:379:LYS:HD2	2:B:422:GLU:HA	1.97	0.45
2:B:450:ILE:HA	3:C:639:PHE:CE2	2.50	0.45
3:F:1111:MET:HG3	3:F:1116:PHE:HZ	1.81	0.45
2:H:207:MET:HA	2:H:210:CYS:SG	2.57	0.45
2:H:450:ILE:HA	3:I:639:PHE:CE2	2.50	0.45
2:K:322:ASN:ND2	2:K:327:TYR:OH	2.31	0.45
2:K:334:LYS:HA	2:K:334:LYS:HD3	1.78	0.45
3:L:548:LYS:HE2	3:L:548:LYS:HB3	1.84	0.45
3:L:771:VAL:HG21	3:L:1000:ALA:HB2	1.98	0.45
2:B:383:MET:CE	2:B:417:MET:HE1	2.46	0.45
2:H:383:MET:CE	2:H:417:MET:HE1	2.46	0.45
2:E:317:PRO:HA	2:E:320:MET:HB2	1.99	0.45
3:F:1009:ALA:HB2	3:F:1018:LEU:HD12	1.97	0.45
3:I:130:LEU:HD22	3:I:177:ASP:HB2	1.98	0.45
2:K:317:PRO:HA	2:K:320:MET:HB2	1.99	0.45
6:K:603:FMN:O2'	6:K:603:FMN:O4'	2.32	0.45
3:L:1111:MET:HG3	3:L:1116:PHE:HZ	1.81	0.45
3:L:15:VAL:HG11	3:L:24:ALA:HB1	1.98	0.45
3:F:148:PRO:HG2	3:F:478:ILE:HG21	1.99	0.45
2:H:186:ASP:HB3	2:H:189:ALA:HB3	1.99	0.45
3:L:148:PRO:HG2	3:L:478:ILE:HG21	1.99	0.45
3:L:1009:ALA:HB2	3:L:1018:LEU:HD12	1.97	0.45
2:B:186:ASP:HB3	2:B:189:ALA:HB3	1.99	0.45
2:E:135:LYS:HD3	2:E:135:LYS:HA	1.80	0.45
2:E:322:ASN:ND2	2:E:327:TYR:OH	2.31	0.45
6:E:603:FMN:O2'	6:E:603:FMN:O4'	2.32	0.45
3:F:15:VAL:HG11	3:F:24:ALA:HB1	1.98	0.45
3:F:443:ASP:HB3	3:F:463:ARG:HD2	1.99	0.45
1:J:24:GLU:O	1:J:28:LYS:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:443:ASP:HB3	3:L:463:ARG:HD2	1.99	0.45
1:D:24:GLU:O	1:D:28:LYS:HB3	2.17	0.45
3:C:15:VAL:HG11	3:C:24:ALA:HB1	1.98	0.44
2:E:383:MET:CE	2:E:417:MET:HE1	2.46	0.44
1:A:135:LEU:HD22	1:A:145:MET:HE2	1.99	0.44
2:K:383:MET:CE	2:K:417:MET:HE1	2.46	0.44
2:B:121:TYR:OH	2:B:205:GLU:OE1	2.23	0.44
3:C:640:ASP:OD1	3:C:640:ASP:N	2.51	0.44
2:E:247:LEU:HD11	2:E:260:MET:HG2	1.99	0.44
1:G:135:LEU:HD22	1:G:145:MET:HE2	1.99	0.44
2:H:121:TYR:OH	2:H:205:GLU:OE1	2.23	0.44
3:I:15:VAL:HG11	3:I:24:ALA:HB1	1.98	0.44
3:I:640:ASP:OD1	3:I:640:ASP:N	2.51	0.44
2:K:450:ILE:HA	3:L:639:PHE:CE2	2.50	0.44
6:E:603:FMN:H1'1	6:E:603:FMN:H9	1.65	0.44
2:H:545:LYS:HD2	2:H:575:VAL:HG21	1.99	0.44
2:B:545:LYS:HD2	2:B:575:VAL:HG21	1.99	0.44
2:E:450:ILE:HA	3:F:639:PHE:CE2	2.50	0.44
3:I:182:GLN:HB3	3:I:251:LEU:HD21	1.99	0.44
3:I:443:ASP:HB3	3:I:463:ARG:HD2	1.99	0.44
2:K:247:LEU:HD11	2:K:260:MET:HG2	1.99	0.44
3:C:182:GLN:HB3	3:C:251:LEU:HD21	1.99	0.44
3:C:443:ASP:HB3	3:C:463:ARG:HD2	1.99	0.44
1:D:135:LEU:HD22	1:D:145:MET:HE2	1.99	0.44
3:F:307:ILE:HD11	3:F:434:GLN:HE22	1.83	0.44
1:J:135:LEU:HD22	1:J:145:MET:HE2	1.99	0.44
3:L:640:ASP:OD1	3:L:640:ASP:N	2.51	0.44
2:E:207:MET:HA	2:E:210:CYS:SG	2.57	0.44
3:F:182:GLN:HB3	3:F:251:LEU:HD21	1.99	0.44
2:K:4:ARG:HB2	2:K:52:ASP:HB2	2.00	0.44
6:K:603:FMN:H1'1	6:K:603:FMN:H9	1.65	0.44
3:L:182:GLN:HB3	3:L:251:LEU:HD21	1.99	0.44
3:L:307:ILE:HD11	3:L:434:GLN:HE22	1.83	0.44
3:C:53:GLU:OE1	3:C:78:THR:HG21	2.18	0.44
3:C:851:HIS:NE2	3:C:936:ASP:OD1	2.46	0.44
2:E:4:ARG:HB2	2:E:52:ASP:HB2	2.00	0.44
3:F:640:ASP:N	3:F:640:ASP:OD1	2.51	0.44
3:I:53:GLU:OE1	3:I:78:THR:HG21	2.18	0.44
3:I:680:GLN:HG2	3:I:711:PHE:HD2	1.83	0.44
3:C:680:GLN:HG2	3:C:711:PHE:HD2	1.83	0.44
1:D:23:LEU:HD13	1:D:48:TYR:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:935:ILE:HG21	3:F:945:VAL:HG22	1.99	0.44
2:K:186:ASP:HB3	2:K:189:ALA:HB3	1.99	0.44
2:B:4:ARG:HB2	2:B:52:ASP:HB2	2.00	0.43
2:E:186:ASP:HB3	2:E:189:ALA:HB3	1.99	0.43
2:E:524:LYS:HA	2:E:524:LYS:HD3	1.86	0.43
2:H:4:ARG:HB2	2:H:52:ASP:HB2	2.00	0.43
1:J:23:LEU:HD13	1:J:48:TYR:HE1	1.83	0.43
2:K:207:MET:HA	2:K:210:CYS:SG	2.57	0.43
3:L:935:ILE:HG21	3:L:945:VAL:HG22	1.99	0.43
2:E:115:PRO:HB2	2:E:233:ARG:HD3	2.00	0.43
3:I:851:HIS:NE2	3:I:936:ASP:OD1	2.46	0.43
1:J:75:THR:HG21	3:L:635:VAL:HG13	2.01	0.43
2:K:115:PRO:HB2	2:K:233:ARG:HD3	2.00	0.43
2:B:317:PRO:HA	2:B:320:MET:HB2	1.99	0.43
3:I:307:ILE:HD11	3:I:434:GLN:HE22	1.83	0.43
3:C:148:PRO:HG2	3:C:478:ILE:HG21	1.99	0.43
1:D:75:THR:HG21	3:F:635:VAL:HG13	2.01	0.43
3:F:53:GLU:OE1	3:F:78:THR:HG21	2.18	0.43
3:I:187:MET:HE2	3:I:187:MET:HB3	1.81	0.43
2:B:438:VAL:HG22	2:B:452:THR:HG23	2.01	0.43
3:C:307:ILE:HD11	3:C:434:GLN:HE22	1.83	0.43
2:E:545:LYS:HD2	2:E:575:VAL:HG21	1.99	0.43
2:H:317:PRO:HA	2:H:320:MET:HB2	1.99	0.43
3:I:675:GLN:CD	3:I:680:GLN:HB2	2.44	0.43
3:I:935:ILE:HG21	3:I:945:VAL:HG22	1.99	0.43
2:K:545:LYS:HD2	2:K:575:VAL:HG21	1.99	0.43
3:L:53:GLU:OE1	3:L:78:THR:HG21	2.18	0.43
1:A:23:LEU:HD13	1:A:48:TYR:HE1	1.83	0.43
3:C:353:TYR:OH	10:C:1203:NDP:O2X	2.37	0.43
3:C:935:ILE:HG21	3:C:945:VAL:HG22	1.99	0.43
3:F:222:GLU:OE2	9:F:1201:FAD:O3B	2.35	0.43
2:H:438:VAL:HG22	2:H:452:THR:HG23	2.01	0.43
3:I:148:PRO:HG2	3:I:478:ILE:HG21	1.99	0.43
3:I:353:TYR:OH	10:I:1203:NDP:O2X	2.37	0.43
3:I:427:ARG:HE	3:I:427:ARG:HB2	1.64	0.43
2:K:524:LYS:HD3	2:K:524:LYS:HA	1.86	0.43
3:L:195:VAL:HG11	3:L:211:LEU:HD13	2.01	0.43
1:A:156:PRO:HA	1:A:159:VAL:HG12	2.00	0.43
3:C:162:GLU:CG	3:C:528:ARG:HB2	2.49	0.43
3:C:675:GLN:CD	3:C:680:GLN:HB2	2.44	0.43
3:C:1159:ASP:O	3:C:1163:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:VAL:HA	1:D:151:TYR:O	2.19	0.43
3:F:195:VAL:HG11	3:F:211:LEU:HD13	2.00	0.43
3:F:675:GLN:CD	3:F:680:GLN:HB2	2.44	0.43
3:I:162:GLU:CG	3:I:528:ARG:HB2	2.49	0.43
3:I:1159:ASP:O	3:I:1163:MET:HG3	2.19	0.43
3:C:187:MET:HE2	3:C:187:MET:HB3	1.81	0.43
3:C:195:VAL:HG11	3:C:211:LEU:HD13	2.00	0.43
1:D:156:PRO:HA	1:D:159:VAL:HG12	2.00	0.43
2:E:129:ALA:HB2	2:E:321:TYR:HB2	2.00	0.43
3:F:162:GLU:CG	3:F:528:ARG:HB2	2.49	0.43
3:F:564:GLU:OE2	3:F:679:LYS:NZ	2.35	0.43
1:G:23:LEU:HD13	1:G:48:TYR:HE1	1.83	0.43
3:I:195:VAL:HG11	3:I:211:LEU:HD13	2.00	0.43
1:J:143:VAL:HA	1:J:151:TYR:O	2.19	0.43
1:J:156:PRO:HA	1:J:159:VAL:HG12	2.00	0.43
2:K:339:LYS:HA	2:K:339:LYS:HD3	1.83	0.43
3:L:287:SER:O	3:L:287:SER:OG	2.36	0.43
3:L:564:GLU:OE2	3:L:679:LYS:NZ	2.35	0.43
3:L:675:GLN:CD	3:L:680:GLN:HB2	2.44	0.43
2:E:334:LYS:HA	2:E:334:LYS:HD3	1.78	0.43
1:G:156:PRO:HA	1:G:159:VAL:HG12	2.00	0.43
2:K:143:ILE:HG12	2:K:165:TRP:HZ3	1.84	0.43
3:L:162:GLU:CG	3:L:528:ARG:HB2	2.49	0.43
3:C:427:ARG:HE	3:C:427:ARG:HB2	1.65	0.43
2:E:143:ILE:HG12	2:E:165:TRP:HZ3	1.84	0.43
3:F:320:THR:HG23	3:F:427:ARG:NH2	2.34	0.43
3:I:320:THR:HG23	3:I:427:ARG:NH2	2.34	0.43
2:K:129:ALA:HB2	2:K:321:TYR:HB2	2.01	0.43
3:L:320:THR:HG23	3:L:427:ARG:NH2	2.34	0.43
3:C:320:THR:HG23	3:C:427:ARG:NH2	2.34	0.42
2:H:135:LYS:HA	2:H:135:LYS:HD3	1.80	0.42
3:I:798:LYS:HD2	3:I:798:LYS:HA	1.83	0.42
3:L:95:ASP:HA	3:L:594:CYS:SG	2.59	0.42
3:L:222:GLU:OE2	9:L:1201:FAD:O3B	2.35	0.42
2:B:129:ALA:HB2	2:B:321:TYR:HB2	2.00	0.42
3:I:746:ILE:HD12	3:I:755:VAL:HG11	2.01	0.42
2:B:135:LYS:HD3	2:B:135:LYS:HA	1.80	0.42
3:C:157:ARG:NH2	3:C:161:GLU:OE2	2.47	0.42
3:C:746:ILE:HD12	3:C:755:VAL:HG11	2.01	0.42
2:E:339:LYS:HA	2:E:339:LYS:HD3	1.83	0.42
3:F:95:ASP:HA	3:F:594:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:ILE:HD11	1:G:65:ASN:CG	2.45	0.42
2:H:129:ALA:HB2	2:H:321:TYR:HB2	2.01	0.42
3:I:157:ARG:NH2	3:I:161:GLU:OE2	2.47	0.42
3:I:1152:PHE:CE2	3:I:1154:GLU:HA	2.54	0.42
1:J:124:ASP:OD1	1:J:124:ASP:N	2.44	0.42
1:A:37:ILE:HD11	1:A:65:ASN:CG	2.45	0.42
1:A:75:THR:HG21	3:C:635:VAL:HG13	2.01	0.42
1:A:101:LEU:HD12	1:A:141:ALA:HB3	2.00	0.42
3:C:831:SER:HA	3:C:1058:ASP:HB2	2.02	0.42
3:C:1152:PHE:CE2	3:C:1154:GLU:HA	2.55	0.42
1:G:75:THR:HG21	3:I:635:VAL:HG13	2.01	0.42
3:I:831:SER:HA	3:I:1058:ASP:HB2	2.02	0.42
2:B:115:PRO:HB2	2:B:233:ARG:HD3	2.00	0.42
3:C:342:LYS:HD2	3:C:342:LYS:HA	1.88	0.42
3:C:798:LYS:HD2	3:C:798:LYS:HA	1.83	0.42
2:E:438:VAL:HG22	2:E:452:THR:HG23	2.01	0.42
3:F:157:ARG:NH2	3:F:161:GLU:OE2	2.47	0.42
3:F:1159:ASP:O	3:F:1163:MET:HG3	2.19	0.42
1:G:101:LEU:HD12	1:G:141:ALA:HB3	2.00	0.42
2:K:438:VAL:HG22	2:K:452:THR:HG23	2.01	0.42
3:L:680:GLN:HG2	3:L:711:PHE:HD2	1.83	0.42
3:L:1159:ASP:O	3:L:1163:MET:HG3	2.19	0.42
1:A:143:VAL:HA	1:A:151:TYR:O	2.19	0.42
2:B:143:ILE:HG12	2:B:165:TRP:HZ3	1.84	0.42
2:B:521:LYS:HA	2:B:527:LEU:HD21	2.02	0.42
1:D:124:ASP:OD1	1:D:124:ASP:N	2.44	0.42
2:H:115:PRO:HB2	2:H:233:ARG:HD3	2.00	0.42
3:I:885:LEU:HD23	3:I:885:LEU:HA	1.88	0.42
2:K:475:LEU:HD23	2:K:475:LEU:HA	1.86	0.42
3:F:680:GLN:HG2	3:F:711:PHE:HD2	1.83	0.42
2:H:521:LYS:HA	2:H:527:LEU:HD21	2.02	0.42
3:I:95:ASP:HA	3:I:594:CYS:SG	2.59	0.42
3:L:157:ARG:NH2	3:L:161:GLU:OE2	2.47	0.42
3:L:353:TYR:OH	10:L:1203:NDP:O2X	2.37	0.42
1:D:101:LEU:HD12	1:D:141:ALA:HB3	2.00	0.42
2:E:121:TYR:OH	2:E:205:GLU:OE1	2.23	0.42
3:F:353:TYR:OH	10:F:1203:NDP:O2X	2.37	0.42
3:F:746:ILE:HD12	3:F:755:VAL:HG11	2.01	0.42
3:F:831:SER:HA	3:F:1058:ASP:HB2	2.02	0.42
3:F:1152:PHE:CE2	3:F:1154:GLU:HA	2.55	0.42
1:G:143:VAL:HA	1:G:151:TYR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:143:ILE:HG12	2:H:165:TRP:HZ3	1.84	0.42
1:J:101:LEU:HD12	1:J:141:ALA:HB3	2.00	0.42
3:L:746:ILE:HD12	3:L:755:VAL:HG11	2.01	0.42
3:L:798:LYS:HD2	3:L:798:LYS:HA	1.83	0.42
3:L:831:SER:HA	3:L:1058:ASP:HB2	2.02	0.42
3:L:1152:PHE:CE2	3:L:1154:GLU:HA	2.55	0.42
3:C:95:ASP:HA	3:C:594:CYS:SG	2.59	0.42
1:D:37:ILE:HD11	1:D:65:ASN:CG	2.45	0.42
1:J:37:ILE:HD11	1:J:65:ASN:CG	2.45	0.42
2:K:121:TYR:OH	2:K:205:GLU:OE1	2.23	0.42
3:C:885:LEU:HD23	3:C:885:LEU:HA	1.88	0.42
2:E:475:LEU:HD23	2:E:475:LEU:HA	1.86	0.42
2:K:439:LYS:HB2	2:K:439:LYS:HE3	1.79	0.42
2:H:55:ASP:HB3	2:H:60:TYR:OH	2.20	0.41
2:H:122:LYS:O	2:H:128:LYS:NZ	2.50	0.41
3:I:39:GLU:H	3:I:39:GLU:CD	2.28	0.41
3:I:342:LYS:HD2	3:I:342:LYS:HA	1.88	0.41
2:B:55:ASP:HB3	2:B:60:TYR:OH	2.20	0.41
2:B:319:ILE:HA	2:B:327:TYR:CE1	2.55	0.41
3:C:39:GLU:H	3:C:39:GLU:CD	2.28	0.41
2:E:439:LYS:HB2	2:E:439:LYS:HE3	1.79	0.41
3:F:798:LYS:HD2	3:F:798:LYS:HA	1.83	0.41
2:E:55:ASP:HB3	2:E:60:TYR:OH	2.20	0.41
2:H:319:ILE:HA	2:H:327:TYR:CE1	2.55	0.41
3:I:387:LEU:HB2	3:I:395:ALA:HB3	2.01	0.41
6:K:603:FMN:N1	6:K:603:FMN:O3'	2.39	0.41
1:A:66:LYS:O	1:A:69:LYS:N	2.51	0.41
3:F:92:LEU:HD23	3:F:92:LEU:HA	1.89	0.41
3:F:848:LYS:HB3	3:F:848:LYS:HE3	1.95	0.41
2:H:164:LYS:HE3	2:H:164:LYS:HB3	1.72	0.41
2:K:55:ASP:HB3	2:K:60:TYR:OH	2.20	0.41
2:B:328:ALA:O	2:B:336:LYS:NZ	2.50	0.41
3:C:373:GLU:O	3:C:540:ASN:ND2	2.54	0.41
3:C:387:LEU:HB2	3:C:395:ALA:HB3	2.01	0.41
2:E:223:CYS:SG	2:E:231:ILE:HD11	2.61	0.41
3:I:373:GLU:O	3:I:540:ASN:ND2	2.54	0.41
2:K:223:CYS:SG	2:K:231:ILE:HD11	2.61	0.41
2:B:223:CYS:SG	2:B:231:ILE:HD11	2.61	0.41
2:E:232:LYS:HA	2:E:235:GLU:HG2	2.02	0.41
3:F:101:ARG:HD3	3:F:105:MET:HE2	2.02	0.41
1:G:66:LYS:O	1:G:69:LYS:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:101:ARG:HD3	3:I:105:MET:HE2	2.02	0.41
2:K:217:ASN:OD1	2:K:217:ASN:N	2.49	0.41
3:L:101:ARG:HD3	3:L:105:MET:HE2	2.02	0.41
3:F:387:LEU:HB2	3:F:395:ALA:HB3	2.01	0.41
2:H:223:CYS:SG	2:H:231:ILE:HD11	2.61	0.41
2:H:328:ALA:O	2:H:336:LYS:NZ	2.50	0.41
3:L:848:LYS:HB3	3:L:848:LYS:HE3	1.95	0.41
3:C:101:ARG:HD3	3:C:105:MET:HE2	2.02	0.41
3:C:407:ASP:HB3	3:C:413:LYS:HE3	2.03	0.41
3:C:536:ALA:HB2	3:C:539:ARG:HH21	1.86	0.41
2:E:217:ASN:OD1	2:E:217:ASN:N	2.49	0.41
2:E:319:ILE:HA	2:E:327:TYR:CE1	2.55	0.41
2:E:521:LYS:HA	2:E:527:LEU:HD21	2.02	0.41
3:F:251:LEU:HD12	3:F:251:LEU:HA	1.91	0.41
3:F:536:ALA:HB2	3:F:539:ARG:HH21	1.86	0.41
3:F:875:THR:HG23	3:F:947:LEU:CD1	2.51	0.41
2:H:548:VAL:HB	7:H:604:SF4:S3	2.61	0.41
3:I:407:ASP:HB3	3:I:413:LYS:HE3	2.03	0.41
1:J:142:PRO:HD2	1:J:154:LEU:H	1.86	0.41
2:K:232:LYS:HA	2:K:235:GLU:HG2	2.03	0.41
2:K:319:ILE:HA	2:K:327:TYR:CE1	2.55	0.41
2:K:521:LYS:HA	2:K:527:LEU:HD21	2.02	0.41
3:L:39:GLU:H	3:L:39:GLU:CD	2.28	0.41
3:L:92:LEU:HD23	3:L:92:LEU:HA	1.89	0.41
3:L:251:LEU:HD12	3:L:251:LEU:HA	1.91	0.41
3:L:387:LEU:HB2	3:L:395:ALA:HB3	2.01	0.41
3:L:536:ALA:HB2	3:L:539:ARG:HH21	1.86	0.41
3:L:875:THR:HG23	3:L:947:LEU:CD1	2.51	0.41
2:B:548:VAL:HB	7:B:604:SF4:S3	2.61	0.41
3:C:158:GLU:HA	3:C:161:GLU:O	2.21	0.41
3:C:548:LYS:HE2	3:C:548:LYS:HB3	1.84	0.41
3:F:39:GLU:H	3:F:39:GLU:CD	2.28	0.41
3:F:787:ARG:HA	3:F:972:ASN:OD1	2.21	0.41
3:I:158:GLU:HA	3:I:161:GLU:O	2.21	0.41
3:I:536:ALA:HB2	3:I:539:ARG:HH21	1.86	0.41
2:B:164:LYS:HE3	2:B:164:LYS:HB3	1.72	0.40
2:B:475:LEU:HA	2:B:475:LEU:HD23	1.86	0.40
3:C:875:THR:HG23	3:C:947:LEU:CD1	2.51	0.40
2:H:298:SER:O	2:H:298:SER:OG	2.37	0.40
3:I:307:ILE:HD13	3:I:307:ILE:HA	1.89	0.40
3:L:373:GLU:O	3:L:540:ASN:ND2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:787:ARG:HA	3:L:972:ASN:OD1	2.21	0.40
2:B:551:ILE:HG12	2:B:561:ILE:HG12	2.04	0.40
1:D:142:PRO:HD2	1:D:154:LEU:H	1.86	0.40
3:F:373:GLU:O	3:F:540:ASN:ND2	2.54	0.40
2:H:232:LYS:HA	2:H:235:GLU:HG2	2.03	0.40
2:H:551:ILE:HG12	2:H:561:ILE:HG12	2.04	0.40
3:I:875:THR:HG23	3:I:947:LEU:CD1	2.51	0.40
1:J:66:LYS:O	1:J:69:LYS:N	2.51	0.40
1:D:66:LYS:O	1:D:69:LYS:N	2.51	0.40
2:E:548:VAL:HB	7:E:604:SF4:S3	2.61	0.40
1:G:140:LEU:HG	1:G:153:LYS:HE3	2.03	0.40
3:I:251:LEU:HD12	3:I:251:LEU:HA	1.91	0.40
1:J:78:SER:OG	2:K:267:GLY:O	2.32	0.40
3:L:860:LEU:HD23	3:L:860:LEU:HA	1.91	0.40
1:A:140:LEU:HG	1:A:153:LYS:HE3	2.03	0.40
2:B:232:LYS:HA	2:B:235:GLU:HG2	2.03	0.40
3:C:251:LEU:HD12	3:C:251:LEU:HA	1.91	0.40
3:C:307:ILE:HD13	3:C:307:ILE:HA	1.89	0.40
3:F:947:LEU:HD23	3:F:947:LEU:HA	1.94	0.40
2:K:548:VAL:HB	7:K:604:SF4:S3	2.61	0.40
2:B:146:ILE:HD13	2:B:146:ILE:HA	1.91	0.40
1:D:140:LEU:HG	1:D:153:LYS:HE3	2.03	0.40
3:F:875:THR:HG23	3:F:947:LEU:HD11	2.04	0.40
1:G:142:PRO:HD2	1:G:154:LEU:H	1.86	0.40
3:I:548:LYS:HE2	3:I:548:LYS:HB3	1.84	0.40
3:I:787:ARG:HA	3:I:972:ASN:OD1	2.21	0.40
1:J:140:LEU:HG	1:J:153:LYS:HE3	2.03	0.40
3:L:158:GLU:HA	3:L:161:GLU:O	2.21	0.40
3:L:307:ILE:HD13	3:L:307:ILE:HA	1.89	0.40
3:L:407:ASP:HB3	3:L:413:LYS:HE3	2.03	0.40
3:L:615:LEU:HD23	3:L:615:LEU:HA	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	148/178 (83%)	138 (93%)	6 (4%)	4 (3%)	4	22
1	D	148/178 (83%)	138 (93%)	6 (4%)	4 (3%)	4	22
1	G	148/178 (83%)	138 (93%)	6 (4%)	4 (3%)	4	22
1	J	148/178 (83%)	138 (93%)	6 (4%)	4 (3%)	4	22
2	B	582/584 (100%)	547 (94%)	33 (6%)	2 (0%)	36	70
2	E	582/584 (100%)	547 (94%)	33 (6%)	2 (0%)	36	70
2	H	582/584 (100%)	547 (94%)	33 (6%)	2 (0%)	36	70
2	K	582/584 (100%)	547 (94%)	33 (6%)	2 (0%)	36	70
3	C	1170/1172 (100%)	1125 (96%)	45 (4%)	0	100	100
3	F	1170/1172 (100%)	1127 (96%)	43 (4%)	0	100	100
3	I	1170/1172 (100%)	1127 (96%)	43 (4%)	0	100	100
3	L	1170/1172 (100%)	1125 (96%)	45 (4%)	0	100	100
All	All	7600/7736 (98%)	7244 (95%)	332 (4%)	24 (0%)	37	70

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	TYR
2	B	524	LYS
1	D	77	TYR
2	E	524	LYS
1	G	77	TYR
2	H	524	LYS
1	J	77	TYR
2	K	524	LYS
1	A	76	PHE
1	A	78	SER
1	D	76	PHE
1	D	78	SER
1	G	76	PHE
1	G	78	SER
1	J	76	PHE
1	J	78	SER
1	A	64	ASP
1	D	64	ASP
1	G	64	ASP

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Mol	Chain	Res	Type
1	J	64	ASP
2	B	228	PRO
2	E	228	PRO
2	H	228	PRO
2	K	228	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	119/142 (84%)	119 (100%)	0	100	100
1	D	119/142 (84%)	119 (100%)	0	100	100
1	G	119/142 (84%)	119 (100%)	0	100	100
1	J	119/142 (84%)	119 (100%)	0	100	100
2	B	471/471 (100%)	468 (99%)	3 (1%)	78	88
2	E	471/471 (100%)	468 (99%)	3 (1%)	78	88
2	H	471/471 (100%)	468 (99%)	3 (1%)	78	88
2	K	471/471 (100%)	468 (99%)	3 (1%)	78	88
3	C	951/951 (100%)	945 (99%)	6 (1%)	78	88
3	F	951/951 (100%)	946 (100%)	5 (0%)	81	89
3	I	951/951 (100%)	947 (100%)	4 (0%)	84	90
3	L	951/951 (100%)	946 (100%)	5 (0%)	81	89
All	All	6164/6256 (98%)	6132 (100%)	32 (0%)	78	89

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	47	TYR
2	B	183	ASP
2	B	184	GLU
3	C	251	LEU
3	C	272	ASP

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Mol	Chain	Res	Type
3	C	583	ASP
3	C	639	PHE
3	C	809	THR
3	C	890	VAL
2	E	47	TYR
2	E	183	ASP
2	E	184	GLU
3	F	251	LEU
3	F	272	ASP
3	F	639	PHE
3	F	809	THR
3	F	890	VAL
2	H	47	TYR
2	H	183	ASP
2	H	184	GLU
3	I	251	LEU
3	I	272	ASP
3	I	639	PHE
3	I	809	THR
2	K	47	TYR
2	K	183	ASP
2	K	184	GLU
3	L	251	LEU
3	L	272	ASP
3	L	583	ASP
3	L	639	PHE
3	L	809	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
2	B	25	GLN
2	B	29	ASN
2	B	306	ASN
3	C	37	HIS
3	C	72	GLN
3	C	125	GLN
3	C	168	GLN
3	C	262	ASN
3	C	545	GLN
3	C	734	HIS

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Mol	Chain	Res	Type
3	C	887	ASN
1	D	83	ASN
2	E	25	GLN
2	E	29	ASN
2	E	306	ASN
3	F	7	ASN
3	F	125	GLN
3	F	168	GLN
3	F	545	GLN
3	F	734	HIS
3	F	887	ASN
3	F	1124	ASN
1	G	83	ASN
2	H	25	GLN
2	H	29	ASN
2	H	306	ASN
3	I	37	HIS
3	I	125	GLN
3	I	168	GLN
3	I	262	ASN
3	I	545	GLN
3	I	734	HIS
3	I	887	ASN
1	J	83	ASN
2	K	25	GLN
2	K	29	ASN
3	L	7	ASN
3	L	125	GLN
3	L	168	GLN
3	L	262	ASN
3	L	545	GLN
3	L	734	HIS
3	L	887	ASN
3	L	1124	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 68 ligands modelled in this entry, 4 are monoatomic - leaving 64 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	FAD	I	1201	-	56,58,58	0.40	1 (1%)	81,89,89	0.38	0
7	SF4	H	605	2	0,12,12	-	-	-		
7	SF4	C	1205	3	0,12,12	-	-	-		
4	FES	F	1209	3	0,4,4	-	-	-		
7	SF4	I	1208	3	0,12,12	-	-	-		
9	FAD	F	1201	-	56,58,58	0.40	1 (1%)	81,89,89	0.38	0
7	SF4	K	604	2	0,12,12	-	-	-		
7	SF4	B	607	2	0,12,12	-	-	-		
7	SF4	B	604	2	0,12,12	-	-	-		
8	NAD	K	606	2	45,48,48	1.68	7 (15%)	63,73,73	2.03	14 (22%)
10	NDP	F	1203	-	49,52,52	1.60	8 (16%)	66,80,80	2.43	22 (33%)
8	NAD	B	606	2	45,48,48	1.68	7 (15%)	63,73,73	2.03	14 (22%)
8	NAD	E	606	2	45,48,48	1.68	7 (15%)	63,73,73	2.03	14 (22%)
7	SF4	H	604	2	0,12,12	-	-	-		
7	SF4	I	1204	3	0,12,12	-	-	-		
9	FAD	C	1201	-	56,58,58	0.40	1 (1%)	81,89,89	0.38	0
7	SF4	B	605	2	0,12,12	-	-	-		
7	SF4	E	605	2	0,12,12	-	-	-		
7	SF4	F	1208	3	0,12,12	-	-	-		
7	SF4	K	605	2	0,12,12	-	-	-		
10	NDP	C	1203	-	49,52,52	1.60	8 (16%)	66,80,80	2.43	22 (33%)
6	FMN	K	603	-	33,33,33	1.11	2 (6%)	48,50,50	1.32	8 (16%)
6	FMN	E	603	-	33,33,33	1.10	2 (6%)	48,50,50	1.32	8 (16%)
7	SF4	F	1204	3	0,12,12	-	-	-		
10	NDP	L	1203	-	49,52,52	1.60	8 (16%)	66,80,80	2.43	22 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	SF4	I	1205	3	0,12,12	-	-	-		
8	NAD	H	606	2	45,48,48	1.68	7 (15%)	63,73,73	2.03	14 (22%)
7	SF4	I	1206	3	0,12,12	-	-	-		
7	SF4	C	1204	3	0,12,12	-	-	-		
7	SF4	E	604	2	0,12,12	-	-	-		
7	SF4	H	607	2	0,12,12	-	-	-		
7	SF4	L	1202	3	0,12,12	-	-	-		
9	FAD	L	1201	-	56,58,58	0.41	1 (1%)	81,89,89	0.38	0
4	FES	I	1209	3	0,4,4	-	-	-		
6	FMN	B	603	-	33,33,33	1.11	2 (6%)	48,50,50	1.32	8 (16%)
4	FES	A	201	1	0,4,4	-	-	-		
4	FES	C	1209	3	0,4,4	-	-	-		
4	FES	J	201	1	0,4,4	-	-	-		
4	FES	L	1209	3	0,4,4	-	-	-		
6	FMN	H	603	-	33,33,33	1.11	2 (6%)	48,50,50	1.31	8 (16%)
7	SF4	L	1207	3	0,12,12	-	-	-		
7	SF4	L	1204	3	0,12,12	-	-	-		
7	SF4	F	1202	3	0,12,12	-	-	-		
4	FES	K	602	2	0,4,4	-	-	-		
4	FES	B	602	2	0,4,4	-	-	-		
7	SF4	L	1206	3	0,12,12	-	-	-		
7	SF4	F	1206	3	0,12,12	-	-	-		
7	SF4	L	1208	3	0,12,12	-	-	-		
10	NDP	I	1203	-	49,52,52	1.59	8 (16%)	66,80,80	2.43	22 (33%)
4	FES	H	602	2	0,4,4	-	-	-		
7	SF4	I	1202	3	0,12,12	-	-	-		
7	SF4	C	1202	3	0,12,12	-	-	-		
7	SF4	F	1207	3	0,12,12	-	-	-		
7	SF4	E	607	2	0,12,12	-	-	-		
7	SF4	K	607	2	0,12,12	-	-	-		
7	SF4	L	1205	3	0,12,12	-	-	-		
4	FES	G	201	1	0,4,4	-	-	-		
7	SF4	C	1206	3	0,12,12	-	-	-		
4	FES	E	602	2	0,4,4	-	-	-		
4	FES	D	201	1	0,4,4	-	-	-		
7	SF4	I	1207	3	0,12,12	-	-	-		
7	SF4	C	1207	3	0,12,12	-	-	-		
7	SF4	F	1205	3	0,12,12	-	-	-		
7	SF4	C	1208	3	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FAD	I	1201	-	-	8/34/50/50	0/6/6/6
7	SF4	H	605	2	-	-	0/6/5/5
7	SF4	C	1205	3	-	-	0/6/5/5
4	FES	F	1209	3	-	-	0/1/1/1
7	SF4	I	1208	3	-	-	0/6/5/5
9	FAD	F	1201	-	-	8/34/50/50	0/6/6/6
7	SF4	K	604	2	-	-	0/6/5/5
7	SF4	B	607	2	-	-	0/6/5/5
7	SF4	B	604	2	-	-	0/6/5/5
8	NAD	K	606	2	-	11/30/62/62	0/5/5/5
10	NDP	F	1203	-	-	12/34/77/77	0/5/5/5
8	NAD	E	606	2	-	11/30/62/62	0/5/5/5
8	NAD	B	606	2	-	11/30/62/62	0/5/5/5
7	SF4	H	604	2	-	-	0/6/5/5
7	SF4	I	1204	3	-	-	0/6/5/5
9	FAD	C	1201	-	-	8/34/50/50	0/6/6/6
7	SF4	B	605	2	-	-	0/6/5/5
10	NDP	C	1203	-	-	12/34/77/77	0/5/5/5
7	SF4	E	605	2	-	-	0/6/5/5
7	SF4	F	1208	3	-	-	0/6/5/5
7	SF4	K	605	2	-	-	0/6/5/5
6	FMN	K	603	-	-	7/18/18/18	0/3/3/3
6	FMN	E	603	-	-	7/18/18/18	0/3/3/3
10	NDP	L	1203	-	-	12/34/77/77	0/5/5/5
7	SF4	F	1204	3	-	-	0/6/5/5
7	SF4	I	1205	3	-	-	0/6/5/5
8	NAD	H	606	2	-	11/30/62/62	0/5/5/5
7	SF4	I	1206	3	-	-	0/6/5/5
9	FAD	L	1201	-	-	8/34/50/50	0/6/6/6
7	SF4	C	1204	3	-	-	0/6/5/5
7	SF4	E	604	2	-	-	0/6/5/5
7	SF4	H	607	2	-	-	0/6/5/5
7	SF4	L	1202	3	-	-	0/6/5/5
4	FES	I	1209	3	-	-	0/1/1/1
6	FMN	B	603	-	-	7/18/18/18	0/3/3/3
4	FES	A	201	1	-	-	0/1/1/1
4	FES	C	1209	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FMN	H	603	-	-	7/18/18/18	0/3/3/3
4	FES	J	201	1	-	-	0/1/1/1
4	FES	L	1209	3	-	-	0/1/1/1
7	SF4	L	1207	3	-	-	0/6/5/5
7	SF4	L	1204	3	-	-	0/6/5/5
7	SF4	F	1202	3	-	-	0/6/5/5
4	FES	B	602	2	-	-	0/1/1/1
4	FES	K	602	2	-	-	0/1/1/1
10	NDP	I	1203	-	-	12/34/77/77	0/5/5/5
7	SF4	F	1206	3	-	-	0/6/5/5
7	SF4	L	1206	3	-	-	0/6/5/5
7	SF4	L	1208	3	-	-	0/6/5/5
4	FES	H	602	2	-	-	0/1/1/1
7	SF4	I	1202	3	-	-	0/6/5/5
7	SF4	C	1202	3	-	-	0/6/5/5
7	SF4	F	1207	3	-	-	0/6/5/5
7	SF4	E	607	2	-	-	0/6/5/5
7	SF4	K	607	2	-	-	0/6/5/5
7	SF4	L	1205	3	-	-	0/6/5/5
4	FES	G	201	1	-	-	0/1/1/1
7	SF4	C	1206	3	-	-	0/6/5/5
4	FES	E	602	2	-	-	0/1/1/1
4	FES	D	201	1	-	-	0/1/1/1
7	SF4	I	1207	3	-	-	0/6/5/5
7	SF4	C	1207	3	-	-	0/6/5/5
7	SF4	F	1205	3	-	-	0/6/5/5
7	SF4	C	1208	3	-	-	0/6/5/5

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	606	NAD	C4N-C3N	6.86	1.51	1.39
8	K	606	NAD	C4N-C3N	6.86	1.51	1.39
8	H	606	NAD	C4N-C3N	6.84	1.51	1.39
8	E	606	NAD	C4N-C3N	6.83	1.51	1.39
10	C	1203	NDP	C5A-C4A	5.86	1.49	1.39
10	F	1203	NDP	C5A-C4A	5.86	1.49	1.39
10	L	1203	NDP	C5A-C4A	5.86	1.49	1.39
10	I	1203	NDP	C5A-C4A	5.82	1.49	1.39
10	I	1203	NDP	C5A-C6A	4.40	1.53	1.41
10	L	1203	NDP	C5A-C6A	4.38	1.53	1.41
10	C	1203	NDP	C5A-C6A	4.37	1.53	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	1203	NDP	C5A-C6A	4.37	1.53	1.41
6	B	603	FMN	C4A-N5	3.73	1.38	1.30
6	K	603	FMN	C4A-N5	3.73	1.38	1.30
6	H	603	FMN	C4A-N5	3.72	1.38	1.30
6	E	603	FMN	C4A-N5	3.69	1.37	1.30
8	B	606	NAD	C5N-C4N	3.62	1.46	1.38
8	E	606	NAD	C5N-C4N	3.62	1.46	1.38
8	H	606	NAD	C5N-C4N	3.61	1.46	1.38
8	K	606	NAD	C5N-C4N	3.61	1.46	1.38
8	B	606	NAD	C5A-C4A	3.52	1.45	1.39
8	E	606	NAD	C5A-C4A	3.52	1.45	1.39
8	H	606	NAD	C5A-C4A	3.52	1.45	1.39
8	K	606	NAD	C5A-C4A	3.52	1.45	1.39
10	L	1203	NDP	C8A-N7A	3.28	1.37	1.31
10	C	1203	NDP	C8A-N7A	3.23	1.37	1.31
10	F	1203	NDP	C8A-N7A	3.23	1.37	1.31
10	I	1203	NDP	C8A-N7A	3.23	1.37	1.31
8	E	606	NAD	C2D-C1D	-3.17	1.48	1.53
8	H	606	NAD	C2D-C1D	-3.14	1.49	1.53
8	B	606	NAD	C2D-C1D	-3.12	1.49	1.53
8	K	606	NAD	C2D-C1D	-3.08	1.49	1.53
10	I	1203	NDP	C6N-C5N	3.01	1.38	1.33
10	C	1203	NDP	C6N-C5N	3.01	1.38	1.33
10	F	1203	NDP	C6N-C5N	3.01	1.38	1.33
10	L	1203	NDP	C6N-C5N	2.97	1.38	1.33
8	B	606	NAD	C5A-N7A	-2.74	1.33	1.39
8	E	606	NAD	C5A-N7A	-2.74	1.33	1.39
8	H	606	NAD	C5A-N7A	-2.74	1.33	1.39
8	K	606	NAD	C5A-N7A	-2.74	1.33	1.39
10	C	1203	NDP	C6A-N6A	2.74	1.41	1.34
10	F	1203	NDP	C6A-N6A	2.74	1.41	1.34
10	L	1203	NDP	C6A-N6A	2.74	1.41	1.34
10	C	1203	NDP	C1B-N9A	2.72	1.54	1.46
10	F	1203	NDP	C1B-N9A	2.72	1.54	1.46
10	L	1203	NDP	C1B-N9A	2.72	1.54	1.46
10	I	1203	NDP	C6A-N6A	2.71	1.40	1.34
10	I	1203	NDP	C1B-N9A	2.70	1.54	1.46
6	H	603	FMN	C10-N1	2.50	1.38	1.33
6	K	603	FMN	C10-N1	2.49	1.38	1.33
6	B	603	FMN	C10-N1	2.46	1.38	1.33
6	E	603	FMN	C10-N1	2.42	1.38	1.33
8	H	606	NAD	C4A-N9A	-2.41	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	606	NAD	C4A-N9A	-2.40	1.32	1.37
8	E	606	NAD	C4A-N9A	-2.40	1.32	1.37
8	K	606	NAD	C4A-N9A	-2.40	1.32	1.37
10	C	1203	NDP	P2B-O2B	2.27	1.63	1.59
10	I	1203	NDP	P2B-O2B	2.27	1.63	1.59
10	F	1203	NDP	P2B-O2B	2.27	1.63	1.59
10	L	1203	NDP	P2B-O2B	2.27	1.63	1.59
10	C	1203	NDP	O7N-C7N	-2.10	1.19	1.24
10	F	1203	NDP	O7N-C7N	-2.10	1.19	1.24
10	I	1203	NDP	O7N-C7N	-2.10	1.19	1.24
10	L	1203	NDP	O7N-C7N	-2.10	1.19	1.24
8	B	606	NAD	C5A-C6A	2.07	1.46	1.41
8	E	606	NAD	C5A-C6A	2.07	1.46	1.41
8	K	606	NAD	C5A-C6A	2.07	1.46	1.41
8	H	606	NAD	C5A-C6A	2.05	1.46	1.41
9	C	1201	FAD	P-O2P	-2.03	1.45	1.55
9	F	1201	FAD	P-O2P	-2.03	1.45	1.55
9	L	1201	FAD	P-O2P	-2.03	1.45	1.55
9	I	1201	FAD	P-O2P	-2.02	1.45	1.55

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	I	1203	NDP	C2B-C1B-N9A	8.81	128.36	113.53
10	L	1203	NDP	C2B-C1B-N9A	8.81	128.36	113.53
10	C	1203	NDP	C2B-C1B-N9A	8.79	128.33	113.53
10	F	1203	NDP	C2B-C1B-N9A	8.79	128.33	113.53
8	E	606	NAD	C5N-C4N-C3N	-7.05	112.00	120.34
8	B	606	NAD	C5N-C4N-C3N	-7.03	112.03	120.34
8	H	606	NAD	C5N-C4N-C3N	-7.02	112.04	120.34
8	K	606	NAD	C5N-C4N-C3N	-6.99	112.07	120.34
10	C	1203	NDP	C4A-C5A-N7A	-6.98	102.12	110.62
10	F	1203	NDP	C4A-C5A-N7A	-6.98	102.12	110.62
10	L	1203	NDP	C4A-C5A-N7A	-6.97	102.13	110.62
10	I	1203	NDP	C4A-C5A-N7A	-6.96	102.14	110.62
10	F	1203	NDP	C5A-C4A-N3A	-6.42	118.38	126.75
10	C	1203	NDP	C5A-C4A-N3A	-6.40	118.40	126.75
10	L	1203	NDP	C5A-C4A-N3A	-6.38	118.42	126.75
10	I	1203	NDP	C5A-C4A-N3A	-6.37	118.44	126.75
8	K	606	NAD	C5A-C4A-N3A	-5.96	118.97	126.75
8	B	606	NAD	C5A-C4A-N3A	-5.95	118.99	126.75
8	E	606	NAD	C5A-C4A-N3A	-5.95	118.99	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	606	NAD	C5A-C4A-N3A	-5.95	118.99	126.75
8	B	606	NAD	C3N-C2N-N1N	4.64	124.96	120.43
8	E	606	NAD	C3N-C2N-N1N	4.64	124.96	120.43
8	K	606	NAD	C3N-C2N-N1N	4.63	124.95	120.43
8	H	606	NAD	C3N-C2N-N1N	4.59	124.92	120.43
10	C	1203	NDP	C5A-C4A-N9A	4.53	111.06	105.78
10	F	1203	NDP	C5A-C4A-N9A	4.53	111.06	105.78
10	L	1203	NDP	C5A-C4A-N9A	4.53	111.06	105.78
10	I	1203	NDP	C5A-C4A-N9A	4.53	111.05	105.78
8	K	606	NAD	N3A-C4A-N9A	4.51	134.52	127.08
8	B	606	NAD	N3A-C4A-N9A	4.50	134.50	127.08
8	E	606	NAD	N3A-C4A-N9A	4.50	134.50	127.08
8	H	606	NAD	N3A-C4A-N9A	4.48	134.47	127.08
10	L	1203	NDP	C5A-N7A-C8A	4.41	109.78	103.51
10	C	1203	NDP	C5A-N7A-C8A	4.41	109.78	103.51
10	F	1203	NDP	C5A-N7A-C8A	4.41	109.78	103.51
10	I	1203	NDP	C5A-N7A-C8A	4.41	109.78	103.51
8	B	606	NAD	C2A-N3A-C4A	3.93	121.04	111.75
8	H	606	NAD	C2A-N3A-C4A	3.93	121.04	111.75
8	K	606	NAD	C2A-N3A-C4A	3.93	121.03	111.75
8	E	606	NAD	C2A-N3A-C4A	3.92	121.01	111.75
10	C	1203	NDP	C5A-C6A-N6A	3.85	131.81	123.43
10	F	1203	NDP	C5A-C6A-N6A	3.85	131.81	123.43
10	I	1203	NDP	C5A-C6A-N6A	3.85	131.80	123.43
10	L	1203	NDP	C6A-C5A-N7A	3.84	139.18	132.02
10	L	1203	NDP	C5A-C6A-N6A	3.84	131.78	123.43
10	C	1203	NDP	C6A-C5A-N7A	3.82	139.15	132.02
10	F	1203	NDP	C6A-C5A-N7A	3.82	139.15	132.02
10	I	1203	NDP	C6A-C5A-N7A	3.82	139.14	132.02
10	I	1203	NDP	C2A-N1A-C6A	3.80	125.29	118.77
10	L	1203	NDP	C2A-N1A-C6A	3.80	125.29	118.77
10	C	1203	NDP	C2A-N1A-C6A	3.79	125.28	118.77
10	F	1203	NDP	C2A-N1A-C6A	3.78	125.25	118.77
10	F	1203	NDP	C2A-N3A-C4A	3.60	120.26	111.75
10	C	1203	NDP	C2A-N3A-C4A	3.59	120.24	111.75
10	I	1203	NDP	C2A-N3A-C4A	3.59	120.23	111.75
10	L	1203	NDP	C2A-N3A-C4A	3.58	120.21	111.75
8	B	606	NAD	N3A-C2A-N1A	-3.52	123.09	128.60
8	H	606	NAD	N3A-C2A-N1A	-3.52	123.09	128.60
8	E	606	NAD	N3A-C2A-N1A	-3.50	123.12	128.60
8	K	606	NAD	N3A-C2A-N1A	-3.50	123.12	128.60
10	I	1203	NDP	O4B-C1B-C2B	-3.49	100.45	106.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	1203	NDP	O4B-C1B-C2B	-3.48	100.47	106.57
10	C	1203	NDP	O4B-C1B-C2B	-3.47	100.48	106.57
10	F	1203	NDP	O4B-C1B-C2B	-3.47	100.48	106.57
6	K	603	FMN	C4-N3-C2	-3.43	119.30	125.64
6	B	603	FMN	C4-N3-C2	-3.41	119.34	125.64
6	H	603	FMN	C4-N3-C2	-3.41	119.34	125.64
6	E	603	FMN	C4-N3-C2	-3.39	119.38	125.64
8	B	606	NAD	O4D-C1D-C2D	-3.31	102.08	106.93
8	E	606	NAD	O4D-C1D-C2D	-3.30	102.10	106.93
8	K	606	NAD	O4D-C1D-C2D	-3.29	102.11	106.93
8	H	606	NAD	C4A-C5A-N7A	-3.29	106.61	110.62
8	K	606	NAD	C4A-C5A-N7A	-3.29	106.61	110.62
8	H	606	NAD	O4D-C1D-C2D	-3.28	102.13	106.93
8	B	606	NAD	C4A-C5A-N7A	-3.26	106.65	110.62
8	E	606	NAD	C4A-C5A-N7A	-3.26	106.65	110.62
10	I	1203	NDP	O4B-C1B-N9A	-3.19	101.78	108.06
10	C	1203	NDP	O4B-C1B-N9A	-3.18	101.80	108.06
10	F	1203	NDP	O4B-C1B-N9A	-3.18	101.80	108.06
10	L	1203	NDP	O4B-C1B-N9A	-3.17	101.82	108.06
8	K	606	NAD	C2N-N1N-C1D	-2.98	112.51	119.14
8	H	606	NAD	C2N-N1N-C1D	-2.97	112.53	119.14
6	K	603	FMN	C4A-C4-N3	2.96	120.71	113.19
8	B	606	NAD	C2N-N1N-C1D	-2.96	112.55	119.14
6	B	603	FMN	C4A-C4-N3	2.95	120.67	113.19
6	H	603	FMN	C4A-C4-N3	2.95	120.67	113.19
8	E	606	NAD	C2N-N1N-C1D	-2.93	112.60	119.14
6	E	603	FMN	C4A-C4-N3	2.93	120.64	113.19
8	K	606	NAD	C5A-N7A-C8A	2.84	107.55	103.51
8	H	606	NAD	C5A-N7A-C8A	2.82	107.52	103.51
8	B	606	NAD	C5A-N7A-C8A	2.81	107.51	103.51
8	E	606	NAD	C5A-N7A-C8A	2.81	107.51	103.51
10	F	1203	NDP	O2B-C2B-C1B	2.75	120.01	110.10
10	I	1203	NDP	O2B-C2B-C1B	2.75	120.01	110.10
10	C	1203	NDP	O2B-C2B-C1B	2.74	119.98	110.10
10	L	1203	NDP	O2B-C2B-C1B	2.74	119.97	110.10
8	B	606	NAD	C4A-N9A-C8A	2.73	108.69	105.73
8	E	606	NAD	C4A-N9A-C8A	2.73	108.69	105.73
8	K	606	NAD	C4A-N9A-C8A	2.73	108.69	105.73
6	K	603	FMN	O4-C4-C4A	-2.70	119.42	126.60
8	H	606	NAD	C4A-N9A-C8A	2.70	108.66	105.73
6	B	603	FMN	O4-C4-C4A	-2.69	119.46	126.60
6	E	603	FMN	O4-C4-C4A	-2.67	119.50	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	603	FMN	O4-C4-C4A	-2.67	119.50	126.60
6	K	603	FMN	C4A-C10-N1	-2.67	118.54	124.73
6	B	603	FMN	C4A-C10-N1	-2.66	118.55	124.73
6	E	603	FMN	C4A-C10-N1	-2.65	118.57	124.73
6	H	603	FMN	C4A-C10-N1	-2.65	118.58	124.73
10	C	1203	NDP	O3B-C3B-C4B	-2.64	103.43	111.05
10	F	1203	NDP	O3B-C3B-C4B	-2.64	103.43	111.05
10	I	1203	NDP	O3B-C3B-C4B	-2.63	103.44	111.05
8	E	606	NAD	C6N-C5N-C4N	2.63	123.26	119.44
10	L	1203	NDP	O3B-C3B-C4B	-2.62	103.46	111.05
8	B	606	NAD	C6N-C5N-C4N	2.59	123.21	119.44
8	H	606	NAD	C6N-C5N-C4N	2.59	123.20	119.44
10	C	1203	NDP	O2B-C2B-C3B	-2.57	102.36	111.68
8	K	606	NAD	C6N-C5N-C4N	2.57	123.18	119.44
10	F	1203	NDP	O2B-C2B-C3B	-2.57	102.36	111.68
10	C	1203	NDP	N3A-C2A-N1A	-2.57	124.58	128.60
10	F	1203	NDP	N3A-C2A-N1A	-2.57	124.58	128.60
10	I	1203	NDP	N3A-C2A-N1A	-2.57	124.58	128.60
10	L	1203	NDP	O2B-C2B-C3B	-2.57	102.37	111.68
10	I	1203	NDP	O2B-C2B-C3B	-2.57	102.37	111.68
10	L	1203	NDP	N3A-C2A-N1A	-2.56	124.59	128.60
6	B	603	FMN	C5A-C9A-N10	2.52	120.56	117.95
6	E	603	FMN	C5A-C9A-N10	2.52	120.56	117.95
6	H	603	FMN	C5A-C9A-N10	2.52	120.56	117.95
6	K	603	FMN	C5A-C9A-N10	2.49	120.53	117.95
8	H	606	NAD	C6A-C5A-N7A	2.45	136.59	132.02
10	L	1203	NDP	O2D-C2D-C1D	2.44	118.17	110.02
10	C	1203	NDP	O2D-C2D-C1D	2.44	118.17	110.02
10	I	1203	NDP	O2D-C2D-C1D	2.43	118.16	110.02
10	F	1203	NDP	O2D-C2D-C1D	2.43	118.14	110.02
8	K	606	NAD	C6A-C5A-N7A	2.42	136.54	132.02
8	B	606	NAD	C6A-C5A-N7A	2.42	136.53	132.02
8	E	606	NAD	C6A-C5A-N7A	2.41	136.50	132.02
8	K	606	NAD	N9A-C8A-N7A	-2.39	110.64	113.91
8	B	606	NAD	N9A-C8A-N7A	-2.39	110.65	113.91
8	E	606	NAD	N9A-C8A-N7A	-2.39	110.65	113.91
8	H	606	NAD	N9A-C8A-N7A	-2.37	110.67	113.91
6	K	603	FMN	C4A-C10-N10	2.34	119.90	116.48
6	H	603	FMN	C4A-C10-N10	2.31	119.86	116.48
6	B	603	FMN	C4A-C10-N10	2.31	119.86	116.48
10	L	1203	NDP	O4B-C4B-C5B	2.30	116.95	109.37
10	C	1203	NDP	O4B-C4B-C5B	2.30	116.93	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	1203	NDP	O4B-C4B-C5B	2.29	116.92	109.37
10	I	1203	NDP	O4B-C4B-C5B	2.29	116.91	109.37
6	E	603	FMN	C4A-C10-N10	2.29	119.83	116.48
6	E	603	FMN	C9A-C5A-N5	-2.27	119.96	122.43
6	B	603	FMN	C10-N1-C2	2.25	121.40	116.90
6	E	603	FMN	C10-N1-C2	2.25	121.39	116.90
6	H	603	FMN	C9A-C5A-N5	-2.24	120.00	122.43
6	K	603	FMN	C10-N1-C2	2.23	121.37	116.90
6	H	603	FMN	C10-N1-C2	2.23	121.37	116.90
10	I	1203	NDP	C4B-O4B-C1B	2.23	114.39	109.47
6	B	603	FMN	C9A-C5A-N5	-2.22	120.02	122.43
10	C	1203	NDP	C4B-O4B-C1B	2.22	114.38	109.47
10	F	1203	NDP	C4B-O4B-C1B	2.22	114.38	109.47
10	L	1203	NDP	C4B-O4B-C1B	2.21	114.36	109.47
10	C	1203	NDP	C1D-N1N-C6N	-2.21	116.06	120.83
10	I	1203	NDP	C1D-N1N-C6N	-2.21	116.06	120.83
10	L	1203	NDP	C1D-N1N-C6N	-2.21	116.06	120.83
6	K	603	FMN	C9A-C5A-N5	-2.21	120.03	122.43
10	F	1203	NDP	C1D-N1N-C6N	-2.20	116.08	120.83
10	I	1203	NDP	C5A-C6A-N1A	-2.17	112.74	117.39
10	I	1203	NDP	PN-O3-PA	-2.17	125.39	132.83
10	F	1203	NDP	PN-O3-PA	-2.16	125.41	132.83
10	C	1203	NDP	PN-O3-PA	-2.16	125.42	132.83
10	C	1203	NDP	C5A-C6A-N1A	-2.16	112.77	117.39
10	L	1203	NDP	PN-O3-PA	-2.15	125.45	132.83
10	L	1203	NDP	C5A-C6A-N1A	-2.15	112.79	117.39
10	F	1203	NDP	C5A-C6A-N1A	-2.15	112.79	117.39
10	F	1203	NDP	N3A-C4A-N9A	2.11	130.57	127.08
10	C	1203	NDP	N3A-C4A-N9A	2.10	130.54	127.08
10	L	1203	NDP	N3A-C4A-N9A	2.09	130.52	127.08
10	I	1203	NDP	N3A-C4A-N9A	2.08	130.51	127.08

There are no chirality outliers.

All (152) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	603	FMN	N10-C1'-C2'-O2'
6	B	603	FMN	N10-C1'-C2'-C3'
6	B	603	FMN	C3'-C4'-C5'-O5'
6	B	603	FMN	O4'-C4'-C5'-O5'
6	E	603	FMN	N10-C1'-C2'-O2'
6	E	603	FMN	N10-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
6	E	603	FMN	C3'-C4'-C5'-O5'
6	E	603	FMN	O4'-C4'-C5'-O5'
6	H	603	FMN	N10-C1'-C2'-O2'
6	H	603	FMN	N10-C1'-C2'-C3'
6	H	603	FMN	C3'-C4'-C5'-O5'
6	H	603	FMN	O4'-C4'-C5'-O5'
6	K	603	FMN	N10-C1'-C2'-O2'
6	K	603	FMN	N10-C1'-C2'-C3'
6	K	603	FMN	C3'-C4'-C5'-O5'
6	K	603	FMN	O4'-C4'-C5'-O5'
8	B	606	NAD	C5B-O5B-PA-O1A
8	B	606	NAD	C5B-O5B-PA-O2A
8	B	606	NAD	O4D-C1D-N1N-C2N
8	B	606	NAD	O4D-C1D-N1N-C6N
8	B	606	NAD	C2D-C1D-N1N-C2N
8	B	606	NAD	C2D-C1D-N1N-C6N
8	E	606	NAD	C5B-O5B-PA-O1A
8	E	606	NAD	C5B-O5B-PA-O2A
8	E	606	NAD	O4D-C1D-N1N-C2N
8	E	606	NAD	O4D-C1D-N1N-C6N
8	E	606	NAD	C2D-C1D-N1N-C2N
8	E	606	NAD	C2D-C1D-N1N-C6N
8	H	606	NAD	C5B-O5B-PA-O1A
8	H	606	NAD	C5B-O5B-PA-O2A
8	H	606	NAD	O4D-C1D-N1N-C2N
8	H	606	NAD	O4D-C1D-N1N-C6N
8	H	606	NAD	C2D-C1D-N1N-C2N
8	H	606	NAD	C2D-C1D-N1N-C6N
8	K	606	NAD	C5B-O5B-PA-O1A
8	K	606	NAD	C5B-O5B-PA-O2A
8	K	606	NAD	O4D-C1D-N1N-C2N
8	K	606	NAD	O4D-C1D-N1N-C6N
8	K	606	NAD	C2D-C1D-N1N-C2N
8	K	606	NAD	C2D-C1D-N1N-C6N
9	C	1201	FAD	C3'-C4'-C5'-O5'
9	C	1201	FAD	O4'-C4'-C5'-O5'
9	C	1201	FAD	C5'-O5'-P-O1P
9	F	1201	FAD	C3'-C4'-C5'-O5'
9	F	1201	FAD	O4'-C4'-C5'-O5'
9	F	1201	FAD	C5'-O5'-P-O1P
9	I	1201	FAD	C3'-C4'-C5'-O5'
9	I	1201	FAD	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
9	I	1201	FAD	C5'-O5'-P-O1P
9	L	1201	FAD	C3'-C4'-C5'-O5'
9	L	1201	FAD	O4'-C4'-C5'-O5'
9	L	1201	FAD	C5'-O5'-P-O1P
10	C	1203	NDP	O4B-C4B-C5B-O5B
10	C	1203	NDP	C3B-C4B-C5B-O5B
10	C	1203	NDP	C5D-O5D-PN-O3
10	C	1203	NDP	C5D-O5D-PN-O1N
10	C	1203	NDP	C5D-O5D-PN-O2N
10	C	1203	NDP	O4D-C4D-C5D-O5D
10	C	1203	NDP	C3D-C4D-C5D-O5D
10	C	1203	NDP	C2N-C3N-C7N-N7N
10	F	1203	NDP	O4B-C4B-C5B-O5B
10	F	1203	NDP	C3B-C4B-C5B-O5B
10	F	1203	NDP	C5D-O5D-PN-O3
10	F	1203	NDP	C5D-O5D-PN-O1N
10	F	1203	NDP	C5D-O5D-PN-O2N
10	F	1203	NDP	O4D-C4D-C5D-O5D
10	F	1203	NDP	C3D-C4D-C5D-O5D
10	F	1203	NDP	C2N-C3N-C7N-N7N
10	I	1203	NDP	O4B-C4B-C5B-O5B
10	I	1203	NDP	C3B-C4B-C5B-O5B
10	I	1203	NDP	C5D-O5D-PN-O3
10	I	1203	NDP	C5D-O5D-PN-O1N
10	I	1203	NDP	C5D-O5D-PN-O2N
10	I	1203	NDP	O4D-C4D-C5D-O5D
10	I	1203	NDP	C3D-C4D-C5D-O5D
10	I	1203	NDP	C2N-C3N-C7N-N7N
10	L	1203	NDP	O4B-C4B-C5B-O5B
10	L	1203	NDP	C3B-C4B-C5B-O5B
10	L	1203	NDP	C5D-O5D-PN-O3
10	L	1203	NDP	C5D-O5D-PN-O1N
10	L	1203	NDP	C5D-O5D-PN-O2N
10	L	1203	NDP	O4D-C4D-C5D-O5D
10	L	1203	NDP	C3D-C4D-C5D-O5D
10	L	1203	NDP	C2N-C3N-C7N-N7N
9	C	1201	FAD	O4B-C4B-C5B-O5B
9	F	1201	FAD	O4B-C4B-C5B-O5B
9	I	1201	FAD	O4B-C4B-C5B-O5B
9	L	1201	FAD	O4B-C4B-C5B-O5B
6	B	603	FMN	C5'-O5'-P-O1P
6	E	603	FMN	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
6	H	603	FMN	C5'-O5'-P-O1P
6	K	603	FMN	C5'-O5'-P-O1P
10	C	1203	NDP	C4D-C5D-O5D-PN
10	F	1203	NDP	C4D-C5D-O5D-PN
10	I	1203	NDP	C4D-C5D-O5D-PN
10	L	1203	NDP	C4D-C5D-O5D-PN
8	B	606	NAD	PA-O3-PN-O1N
8	E	606	NAD	PA-O3-PN-O1N
8	H	606	NAD	PA-O3-PN-O1N
8	K	606	NAD	PA-O3-PN-O1N
8	B	606	NAD	O4B-C4B-C5B-O5B
8	E	606	NAD	O4B-C4B-C5B-O5B
8	H	606	NAD	O4B-C4B-C5B-O5B
8	K	606	NAD	O4B-C4B-C5B-O5B
9	C	1201	FAD	C3B-C4B-C5B-O5B
9	F	1201	FAD	C3B-C4B-C5B-O5B
9	I	1201	FAD	C3B-C4B-C5B-O5B
9	L	1201	FAD	C3B-C4B-C5B-O5B
8	B	606	NAD	PA-O3-PN-O5D
8	E	606	NAD	PA-O3-PN-O5D
8	H	606	NAD	PA-O3-PN-O5D
8	K	606	NAD	PA-O3-PN-O5D
9	C	1201	FAD	PA-O3P-P-O5'
9	F	1201	FAD	PA-O3P-P-O5'
9	I	1201	FAD	PA-O3P-P-O5'
9	L	1201	FAD	PA-O3P-P-O5'
9	C	1201	FAD	C5'-O5'-P-O3P
9	F	1201	FAD	C5'-O5'-P-O3P
9	I	1201	FAD	C5'-O5'-P-O3P
9	L	1201	FAD	C5'-O5'-P-O3P
8	B	606	NAD	C3B-C4B-C5B-O5B
8	E	606	NAD	C3B-C4B-C5B-O5B
8	H	606	NAD	C3B-C4B-C5B-O5B
8	K	606	NAD	C3B-C4B-C5B-O5B
10	C	1203	NDP	O4D-C1D-N1N-C6N
10	F	1203	NDP	O4D-C1D-N1N-C6N
10	I	1203	NDP	O4D-C1D-N1N-C6N
10	L	1203	NDP	O4D-C1D-N1N-C6N
9	C	1201	FAD	C5'-O5'-P-O2P
9	F	1201	FAD	C5'-O5'-P-O2P
9	I	1201	FAD	C5'-O5'-P-O2P
9	L	1201	FAD	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
10	C	1203	NDP	PN-O3-PA-O2A
10	F	1203	NDP	PN-O3-PA-O2A
10	I	1203	NDP	PN-O3-PA-O2A
10	L	1203	NDP	PN-O3-PA-O2A
6	B	603	FMN	C2'-C1'-N10-C10
6	E	603	FMN	C2'-C1'-N10-C10
6	H	603	FMN	C2'-C1'-N10-C10
6	K	603	FMN	C2'-C1'-N10-C10
6	B	603	FMN	C5'-O5'-P-O2P
6	E	603	FMN	C5'-O5'-P-O2P
6	H	603	FMN	C5'-O5'-P-O2P
6	K	603	FMN	C5'-O5'-P-O2P
8	B	606	NAD	C5B-O5B-PA-O3
8	E	606	NAD	C5B-O5B-PA-O3
8	H	606	NAD	C5B-O5B-PA-O3
8	K	606	NAD	C5B-O5B-PA-O3
10	C	1203	NDP	PN-O3-PA-O1A
10	F	1203	NDP	PN-O3-PA-O1A
10	I	1203	NDP	PN-O3-PA-O1A
10	L	1203	NDP	PN-O3-PA-O1A

There are no ring outliers.

22 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	1201	FAD	1	0
7	K	604	SF4	2	0
7	B	604	SF4	2	0
8	K	606	NAD	3	0
10	F	1203	NDP	6	0
8	B	606	NAD	3	0
8	E	606	NAD	3	0
7	H	604	SF4	2	0
10	C	1203	NDP	6	0
6	K	603	FMN	5	0
6	E	603	FMN	4	0
10	L	1203	NDP	6	0
8	H	606	NAD	3	0
7	I	1206	SF4	1	0
7	E	604	SF4	2	0
9	L	1201	FAD	1	0
6	B	603	FMN	3	0

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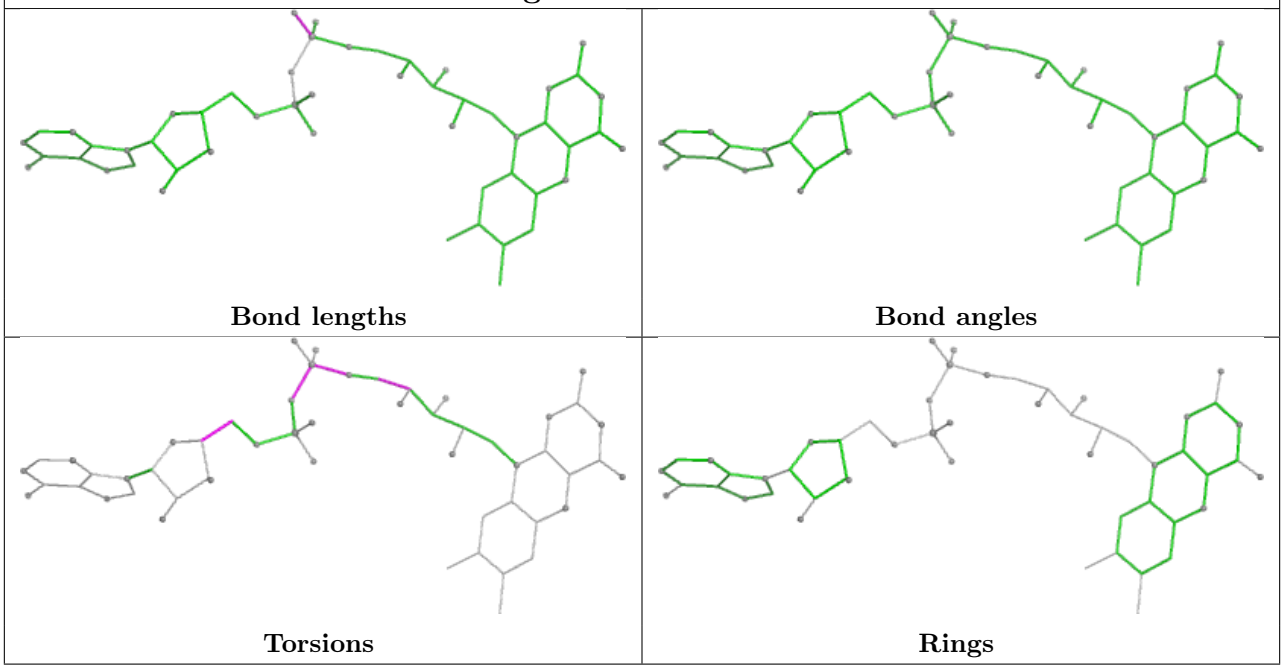
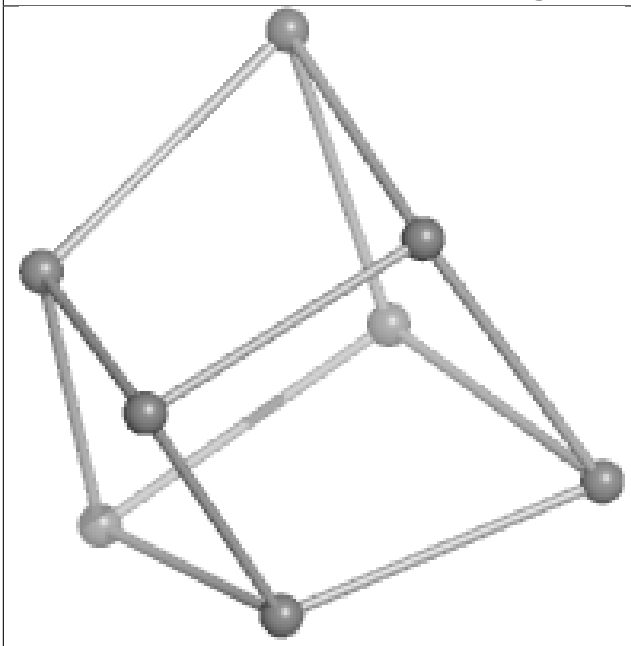
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	603	FMN	3	0
7	L	1206	SF4	1	0
7	F	1206	SF4	1	0
10	I	1203	NDP	6	0
7	C	1206	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

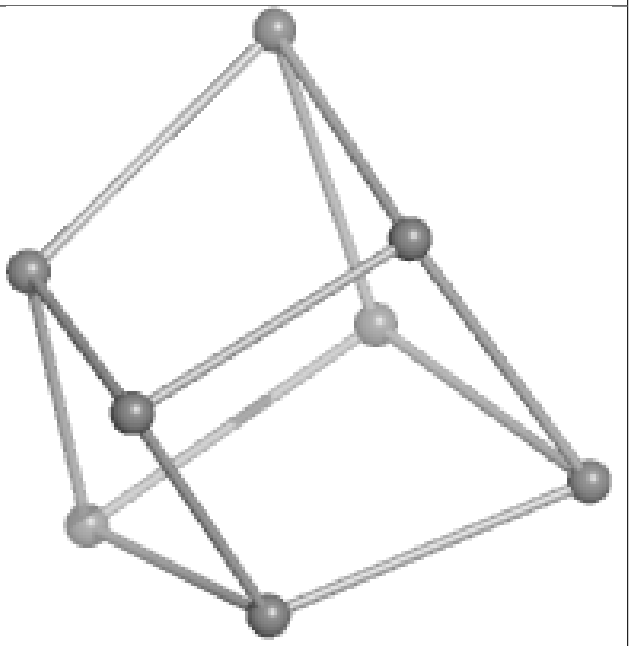
Ligand FAD I 1201



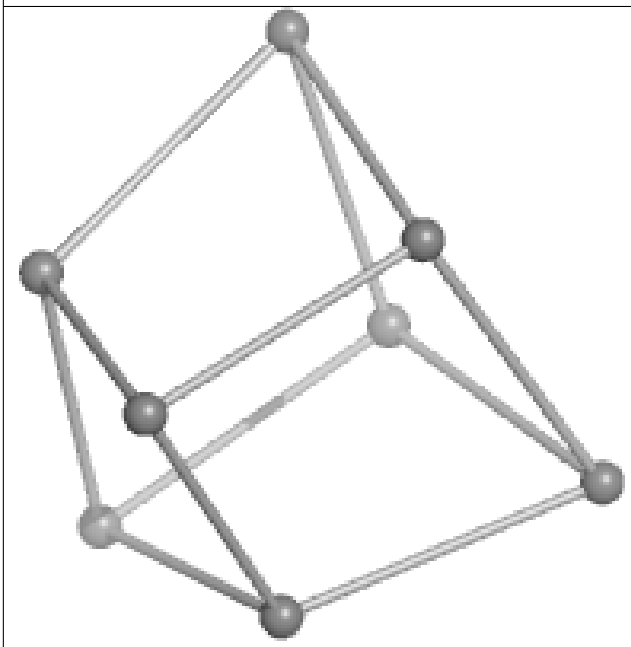
Ligand SF4 H 605



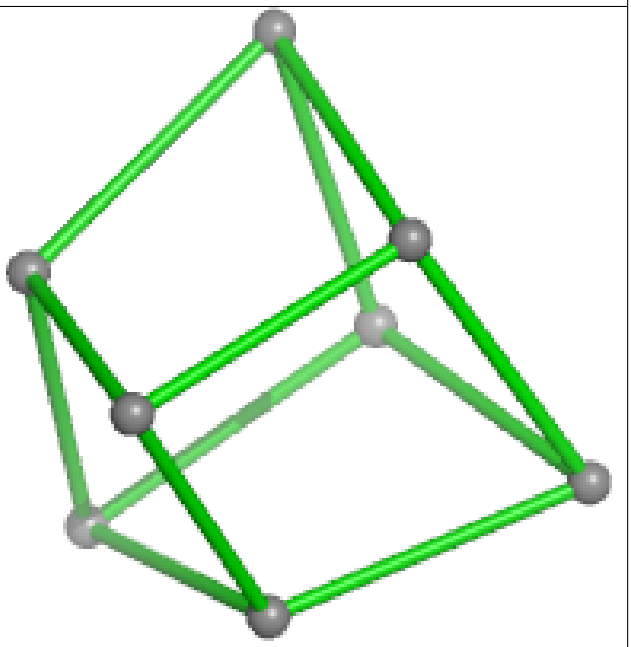
Bond lengths



Bond angles

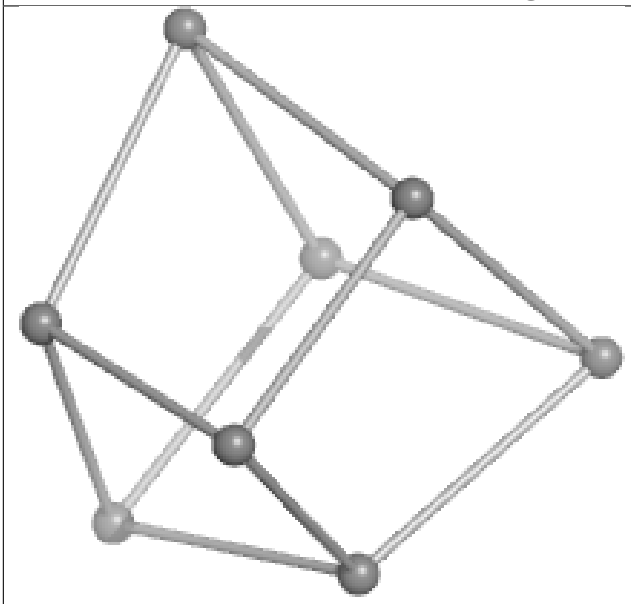


Torsions

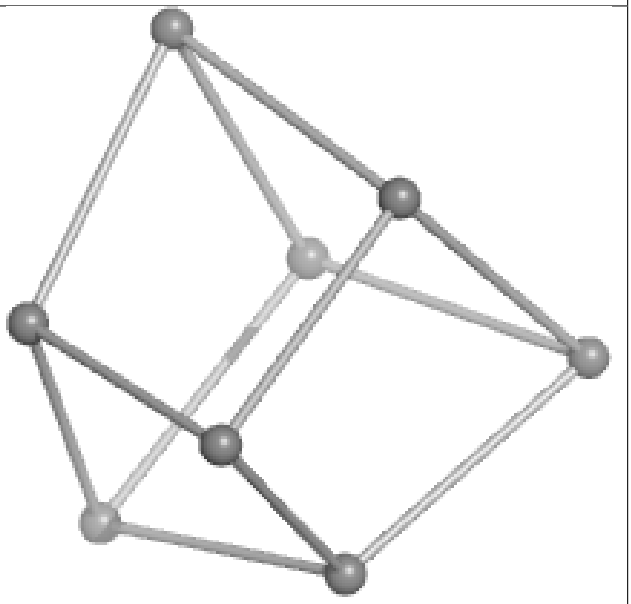


Rings

Ligand SF4 C 1205



Bond lengths



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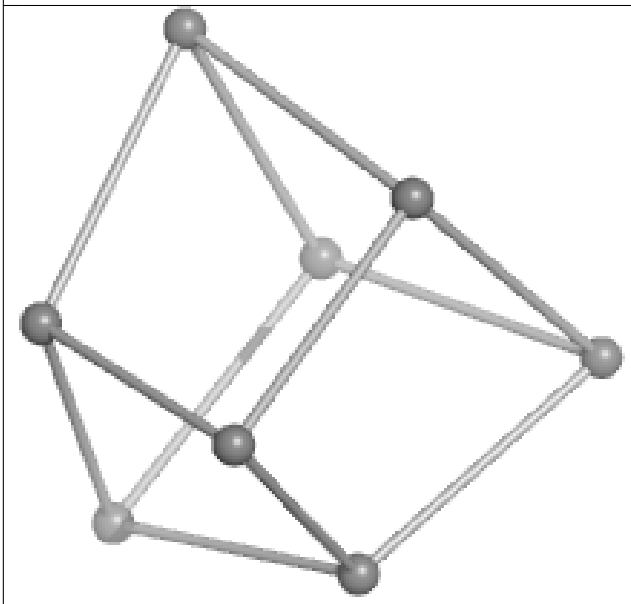
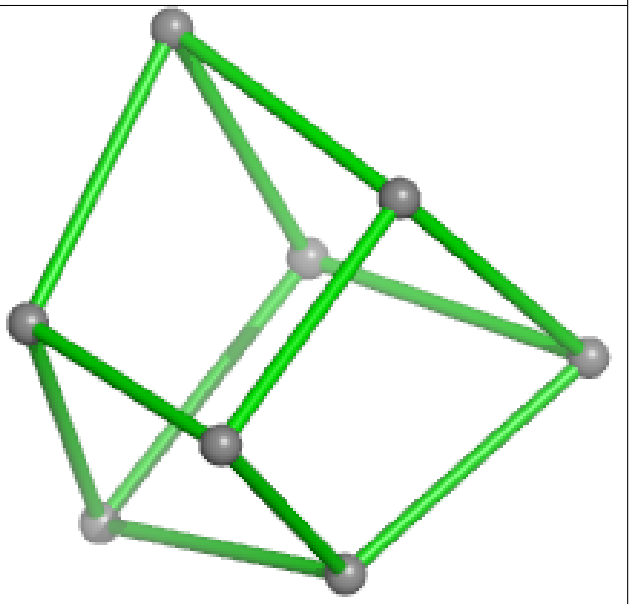
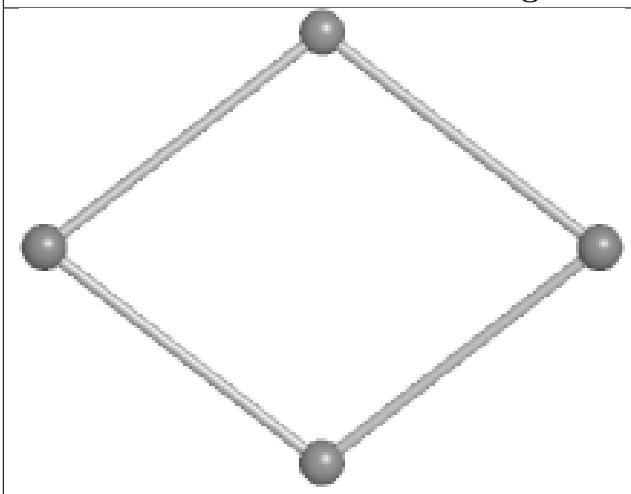


Torsions

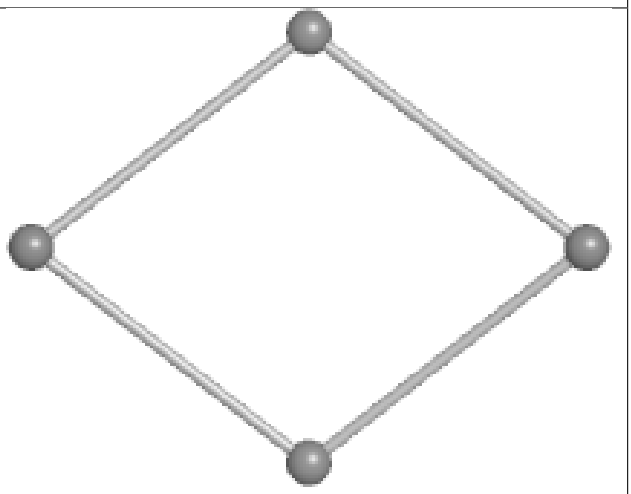


Rings

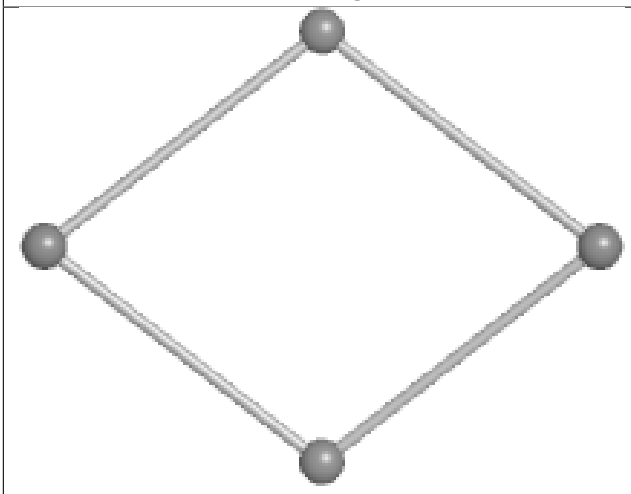
Ligand FES F 1209



Bond lengths



Bond angles



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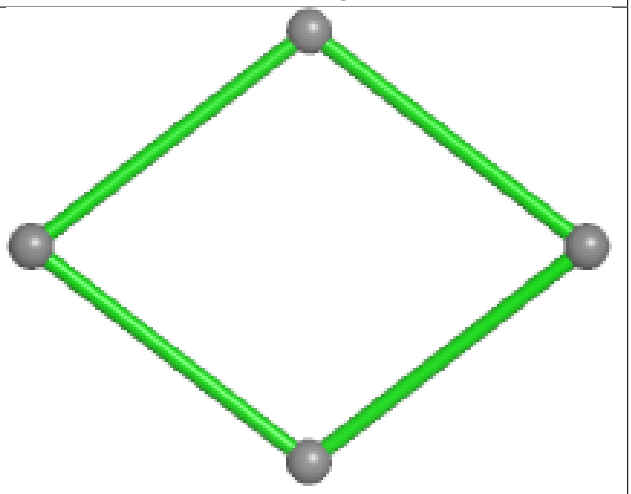
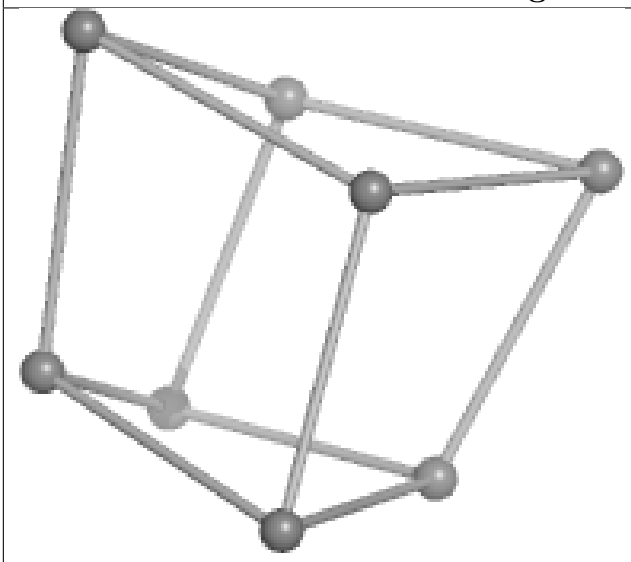


Rings

Ligand SF4 I 1208



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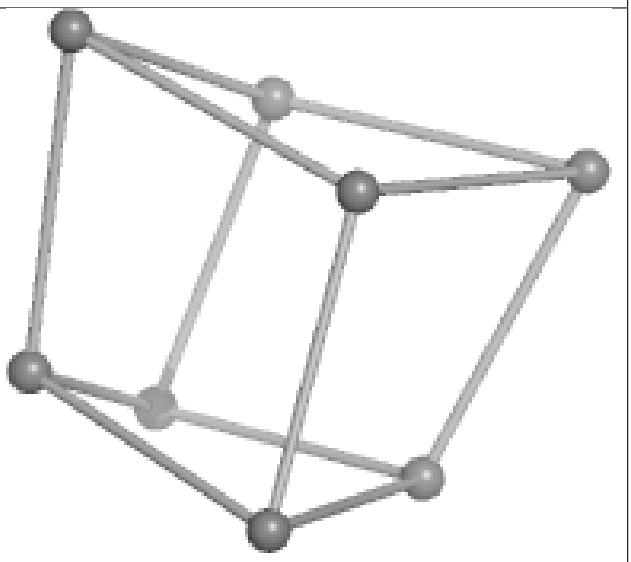
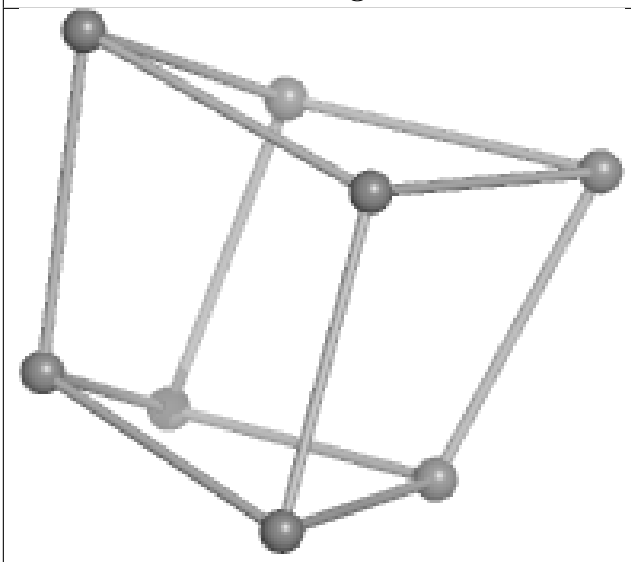


Bond angles



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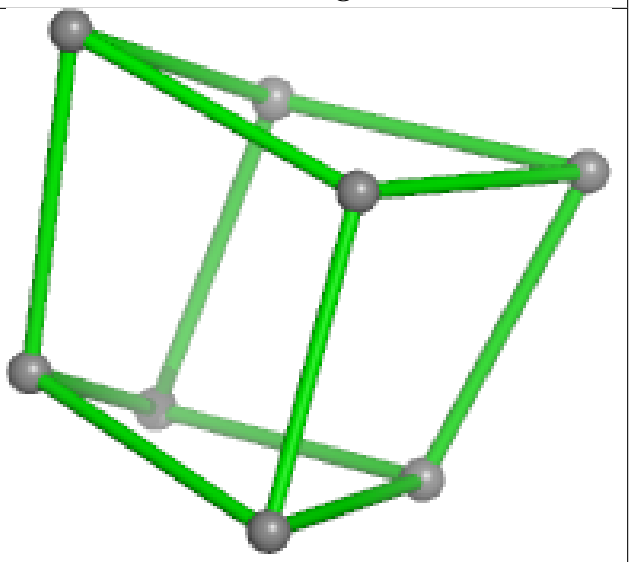
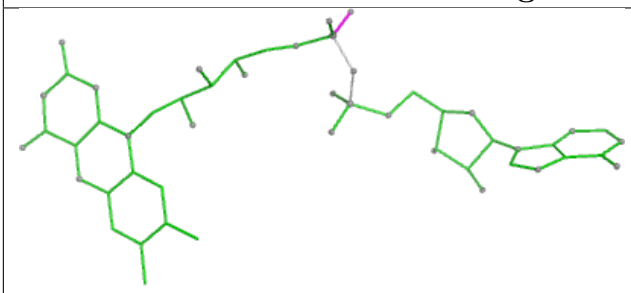


Rings

Ligand FAD F 1201



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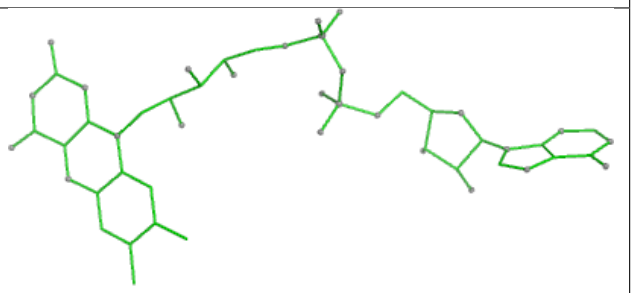
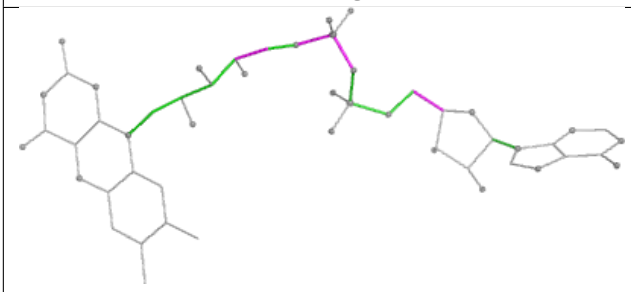


Bond angles



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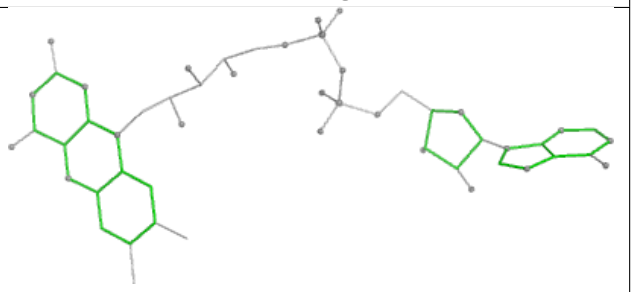
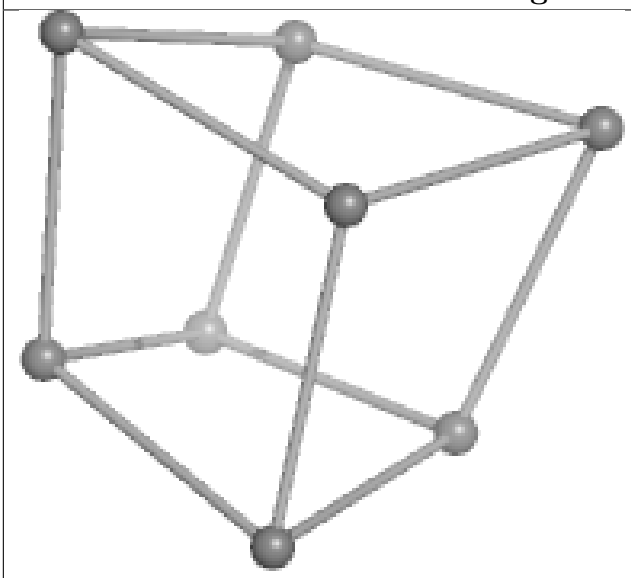


Rings

Ligand SF4 K 604



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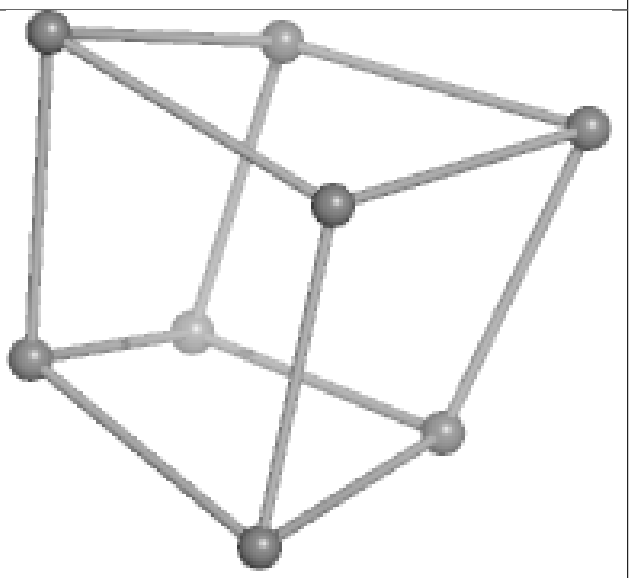
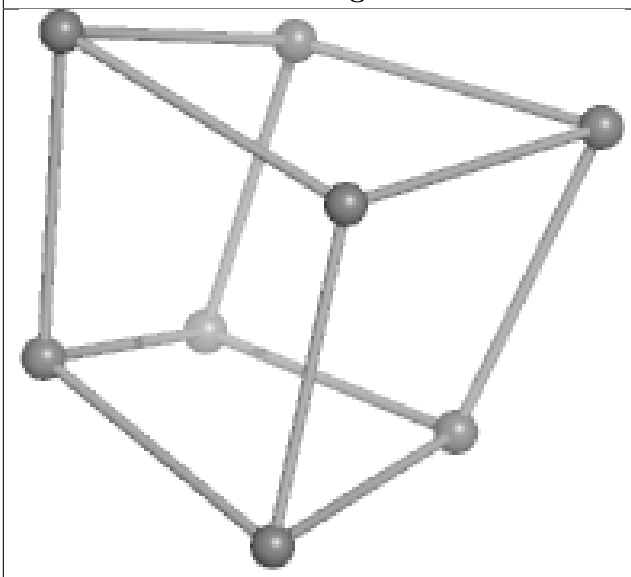
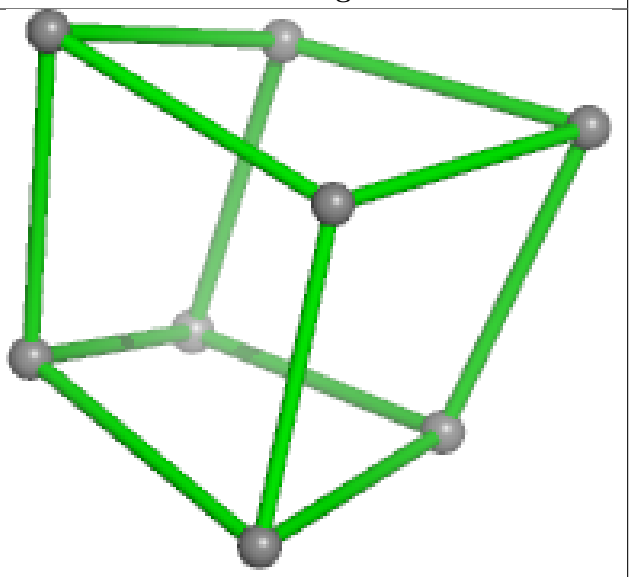


Bond angles

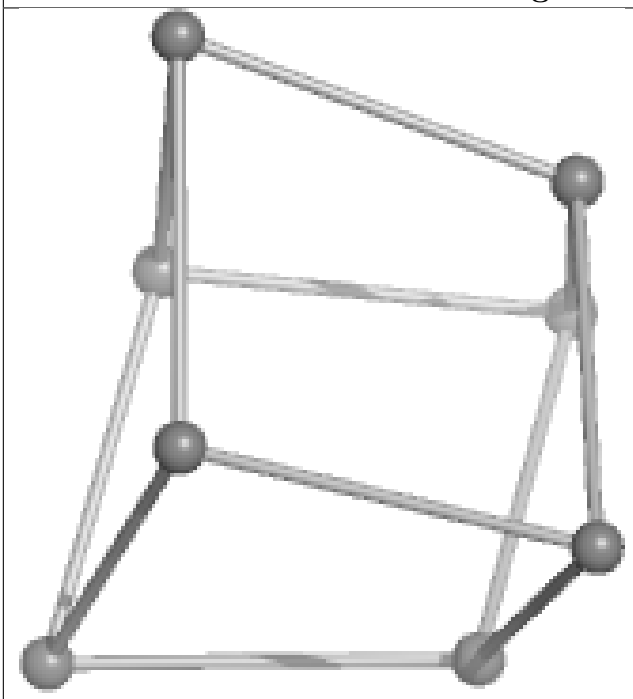


Torsions

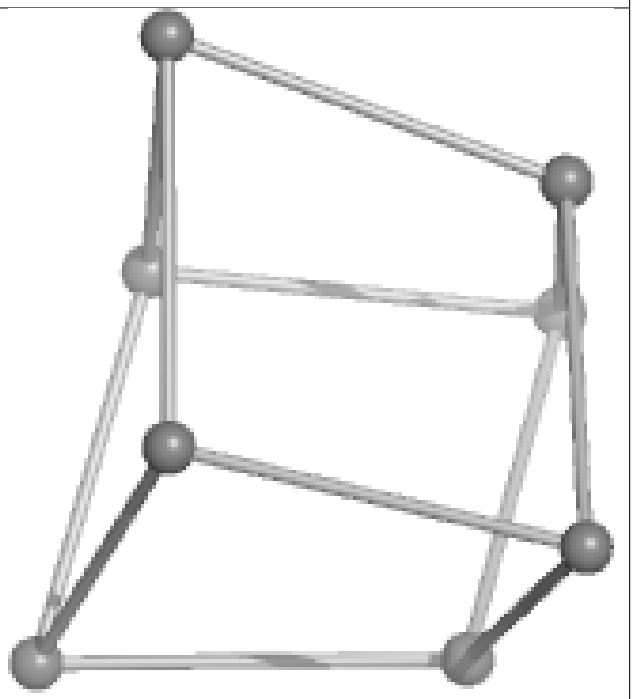


Rings

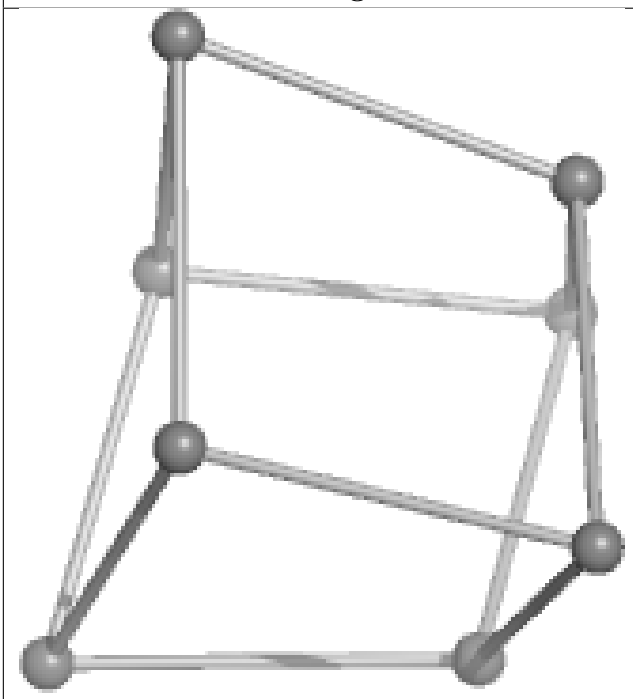
Ligand SF4 B 607



Bond lengths



Bond angles



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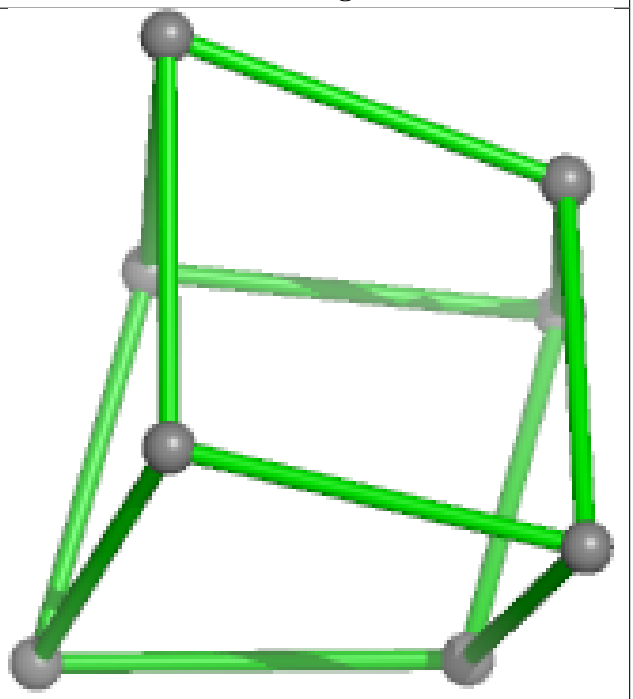
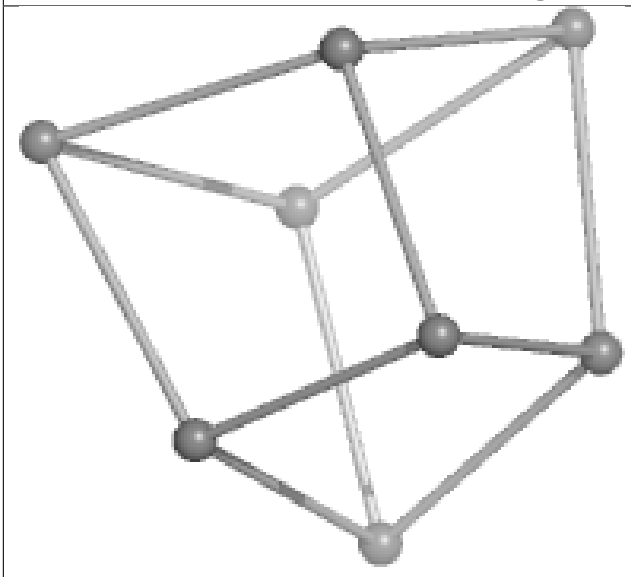


Rings

Ligand SF4 B 604



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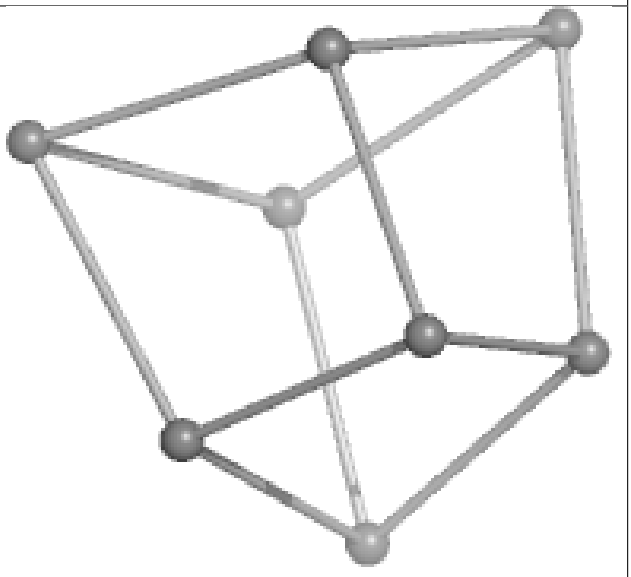

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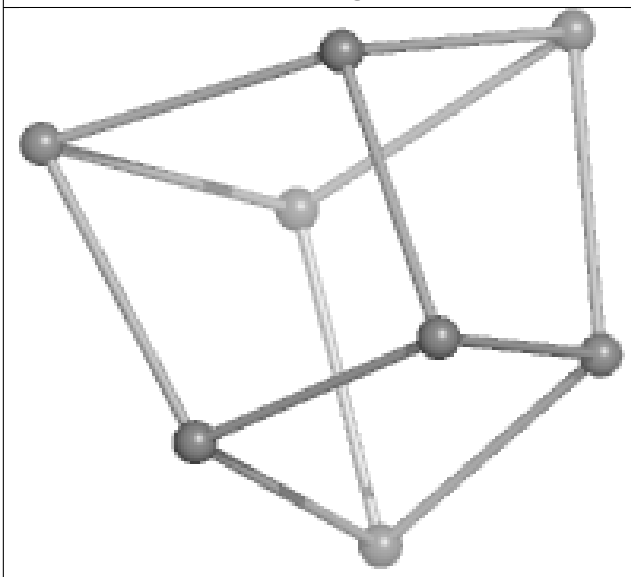

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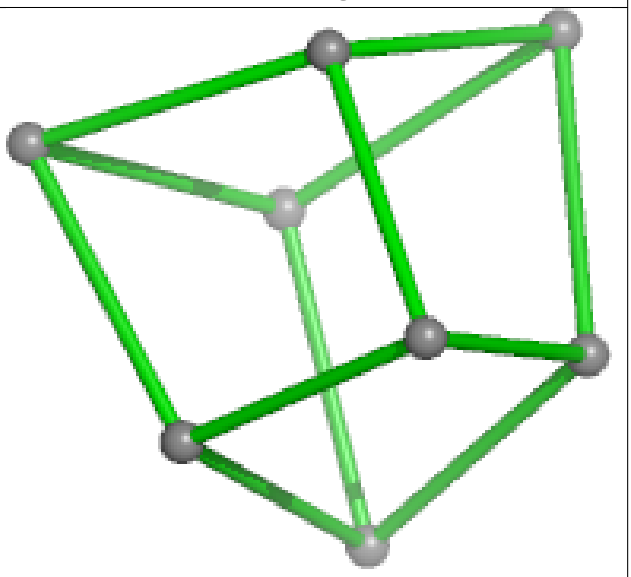
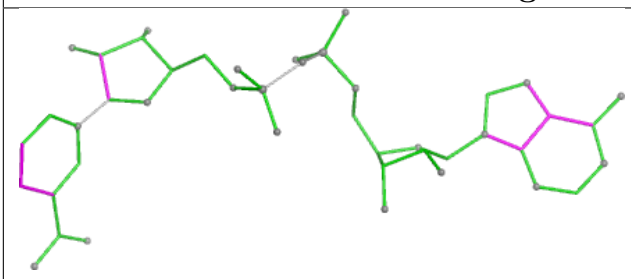


Rings

Ligand NAD K 606



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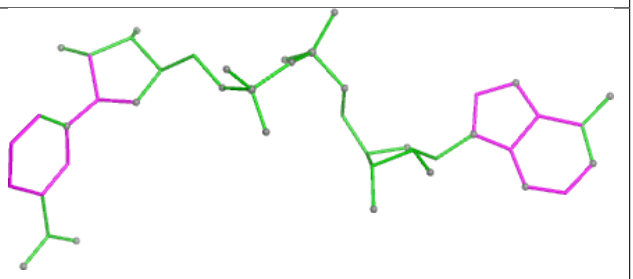

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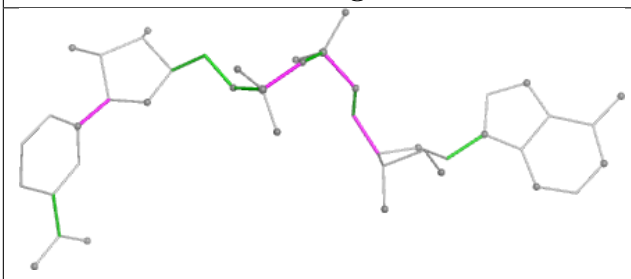

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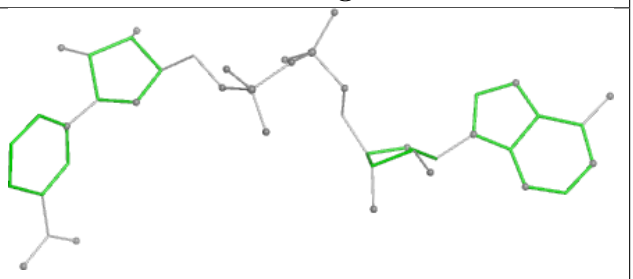
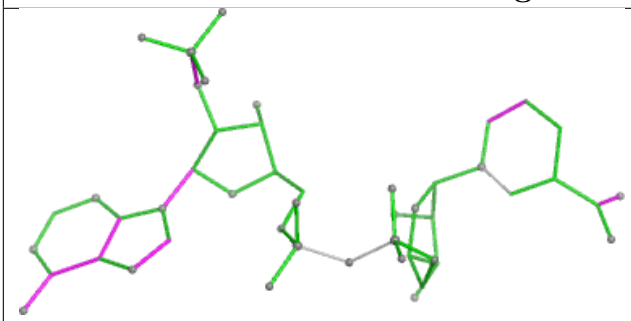


Rings

Ligand NDP F 1203



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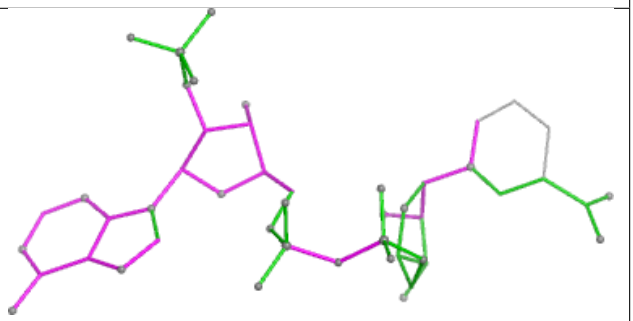

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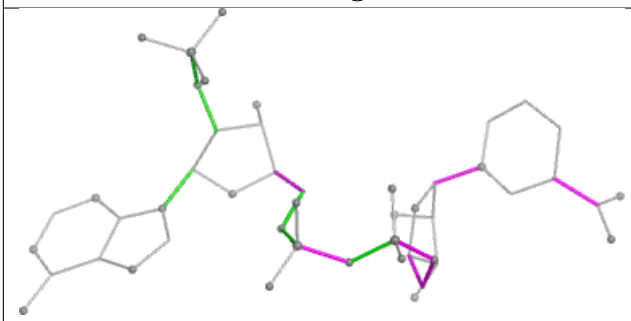

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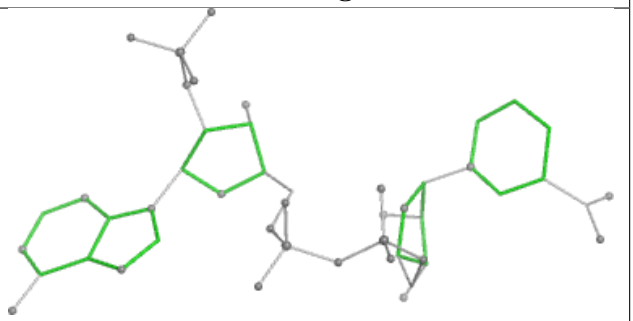
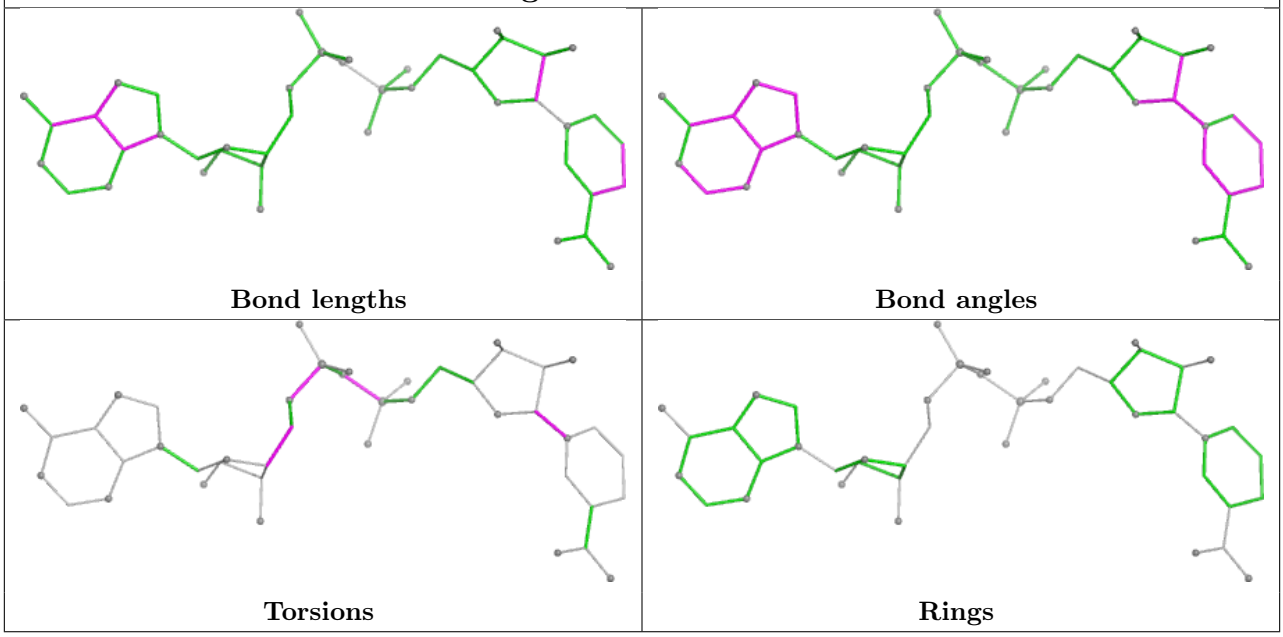


Rings

Ligand NAD B 606



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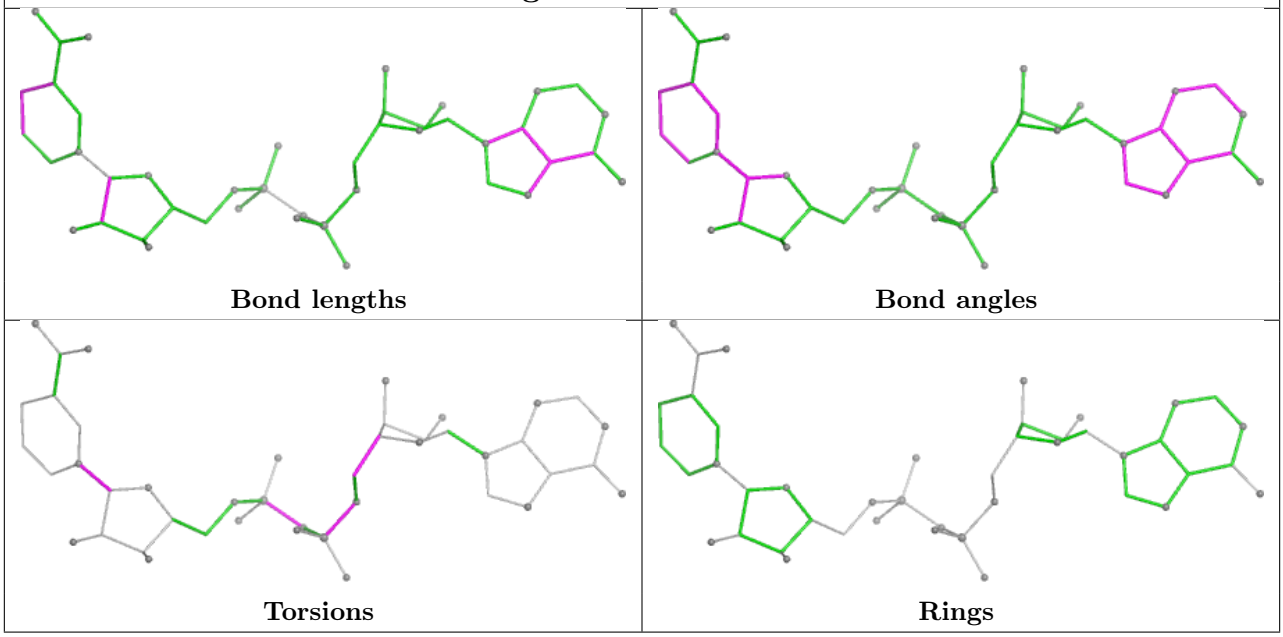
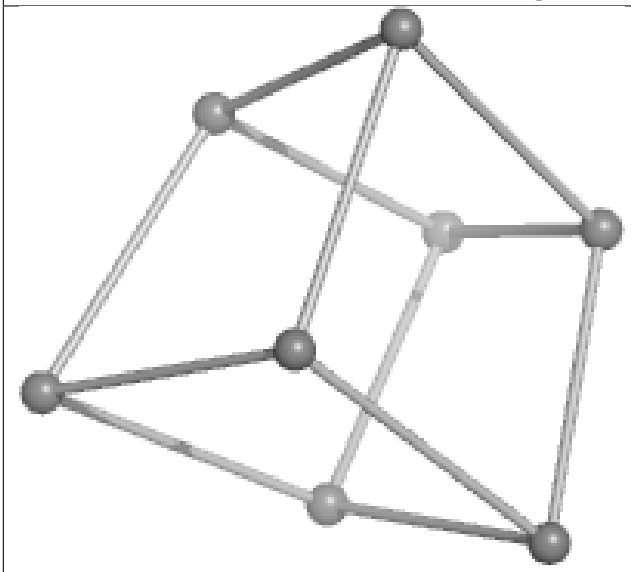


Ligand SF4 H 604



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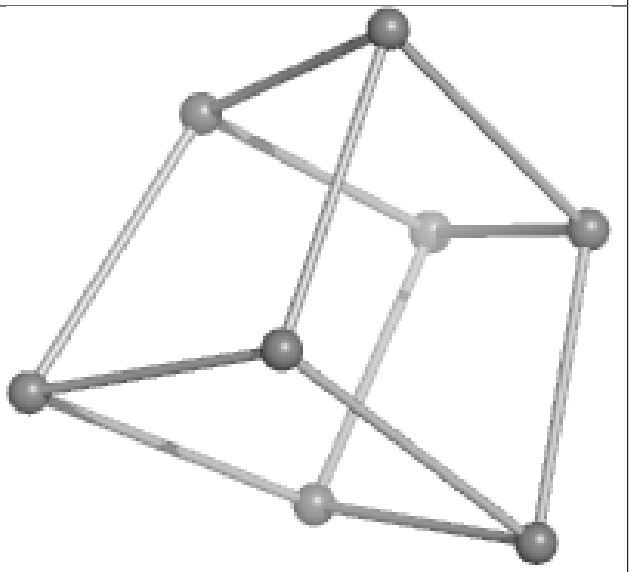

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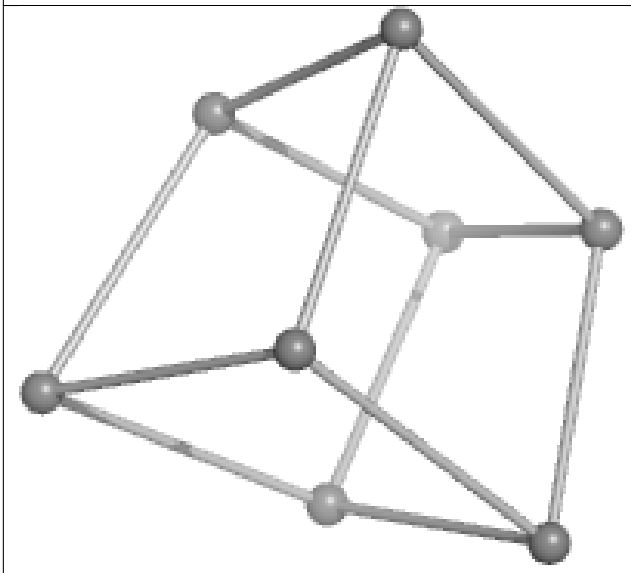

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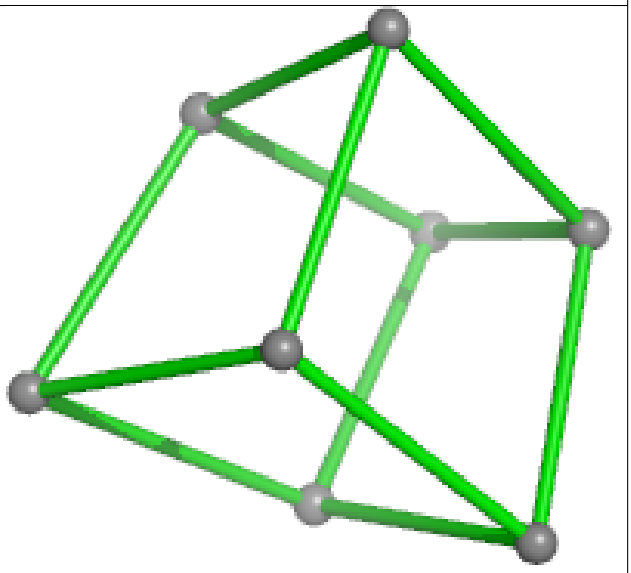
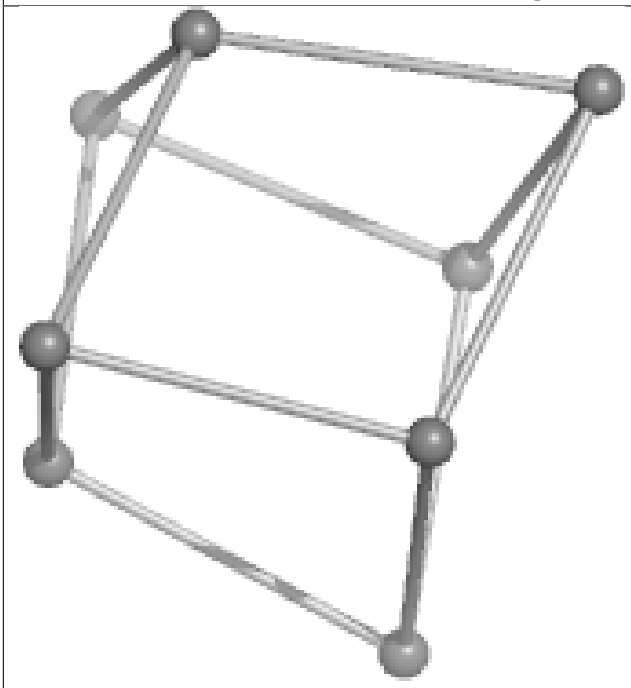


Rings

Ligand SF4 I 1204



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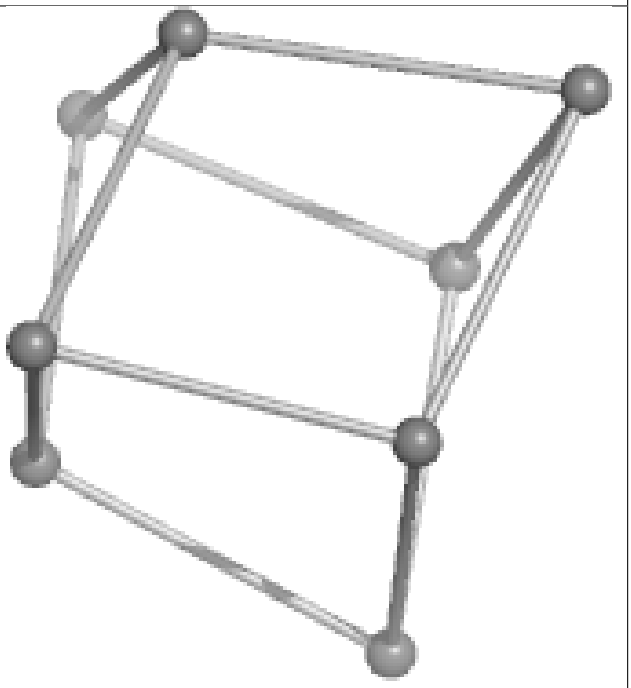

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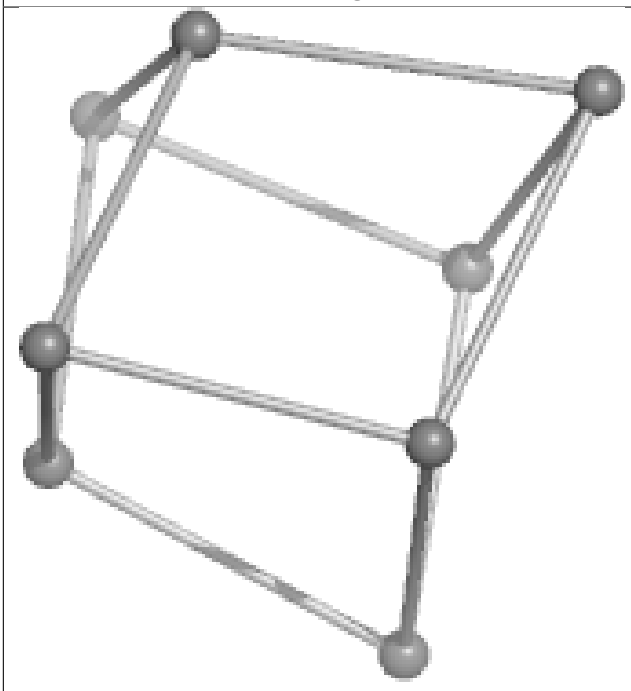

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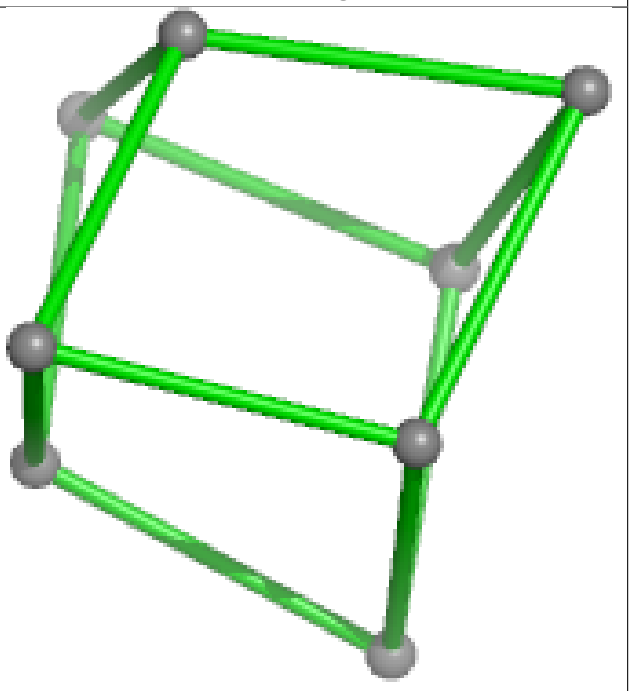
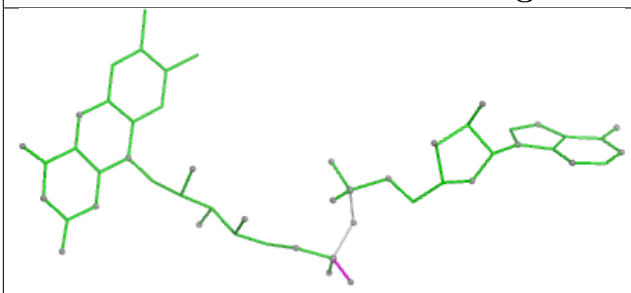


Rings

Ligand FAD C 1201



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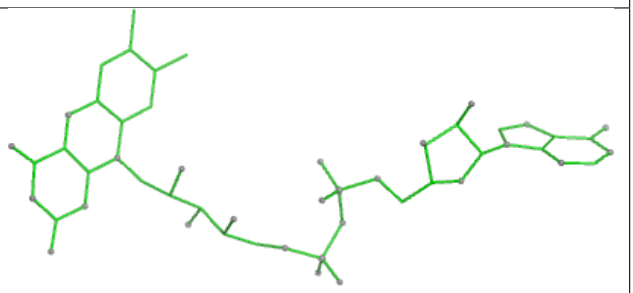

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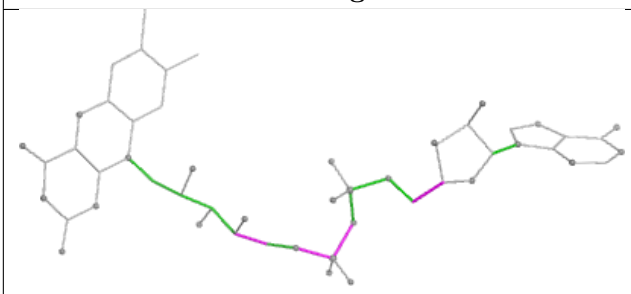

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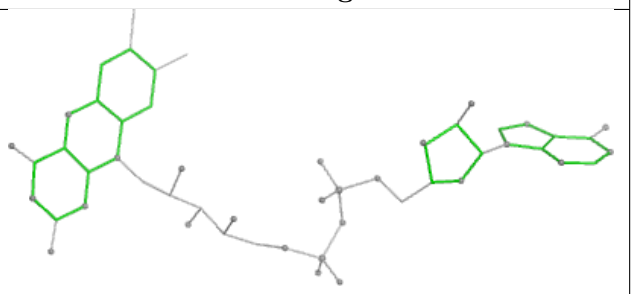
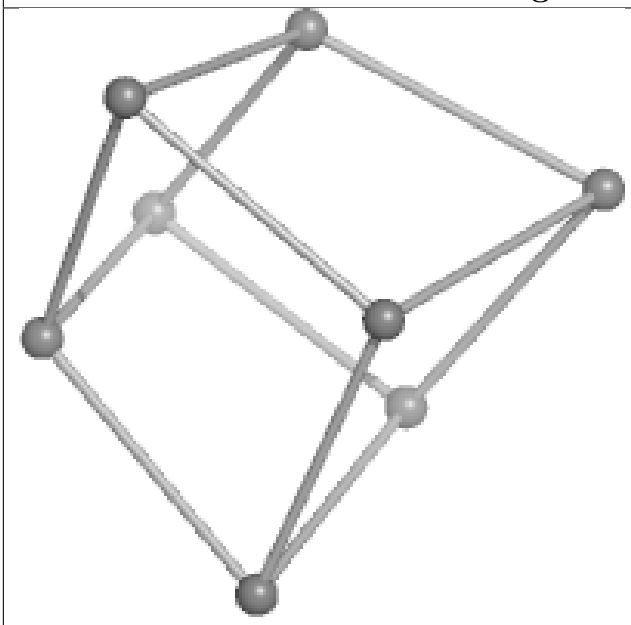


Rings

Ligand SF4 B 605



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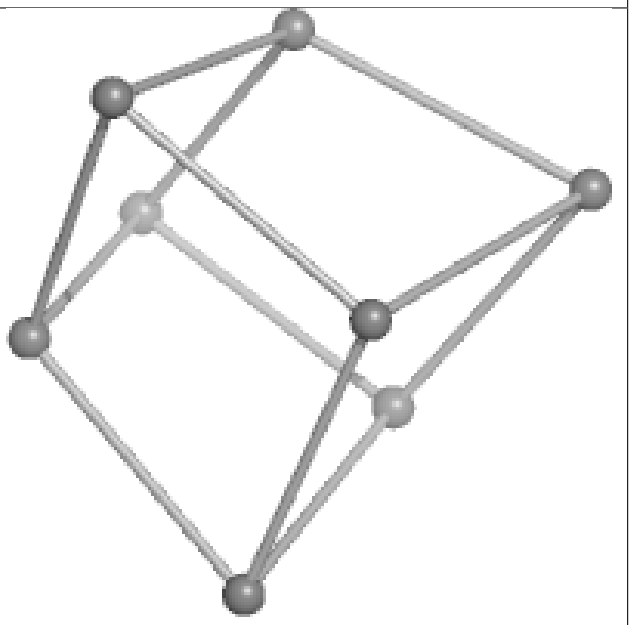

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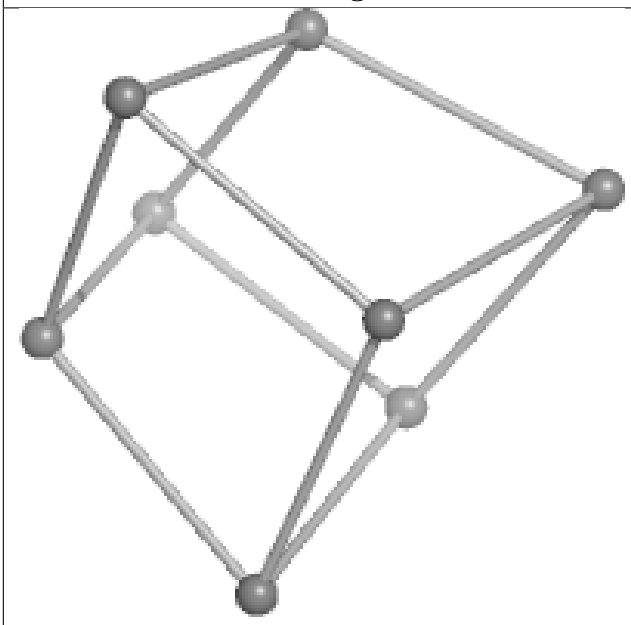

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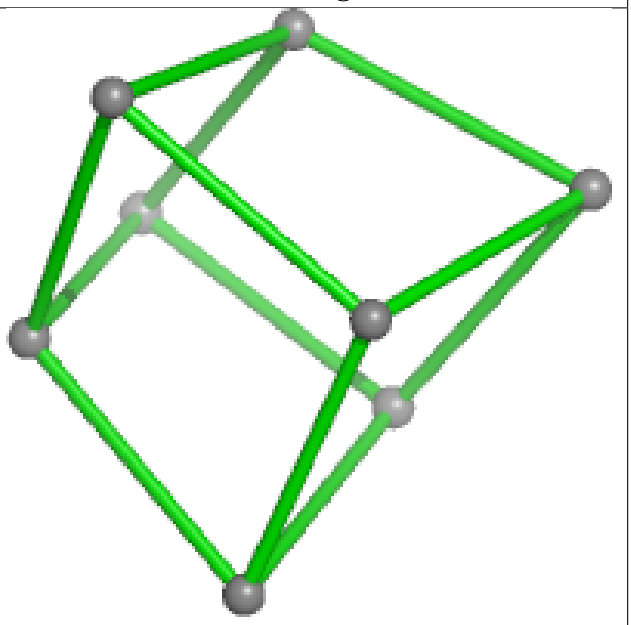
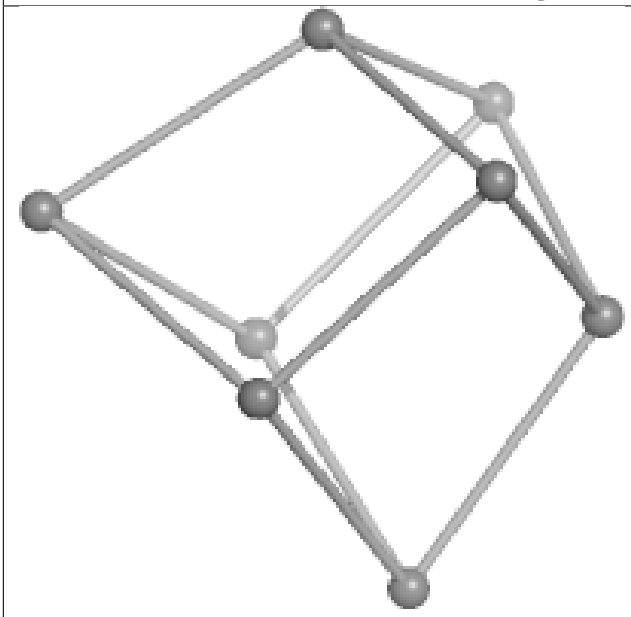


Rings

Ligand SF4 E 605



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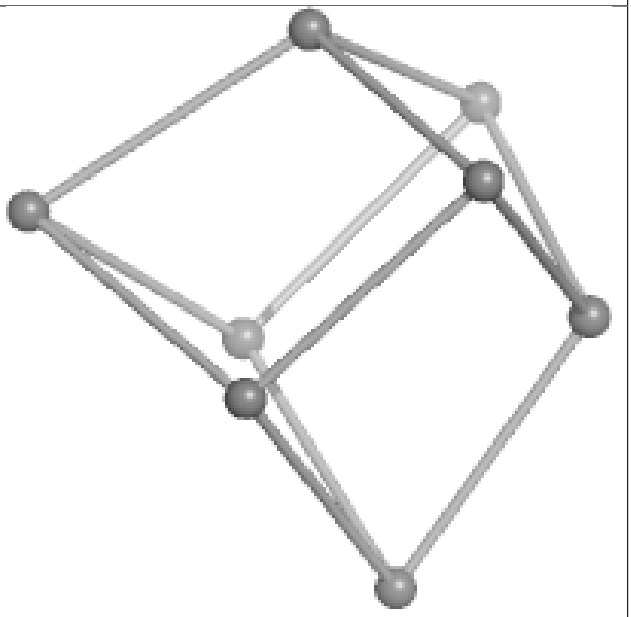

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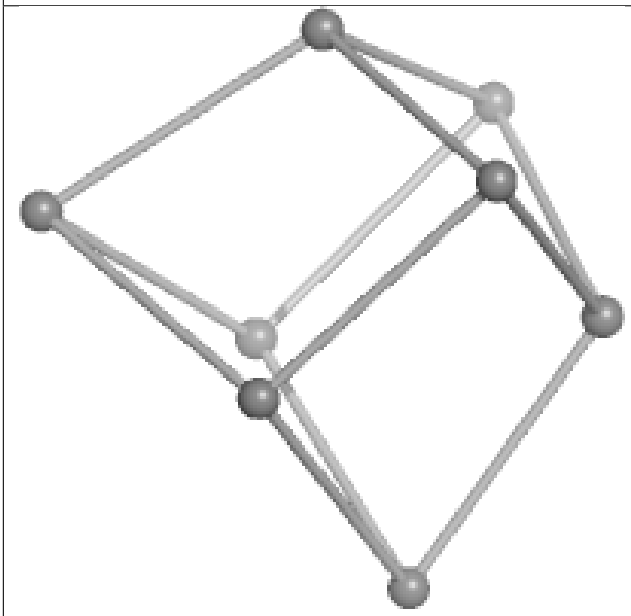

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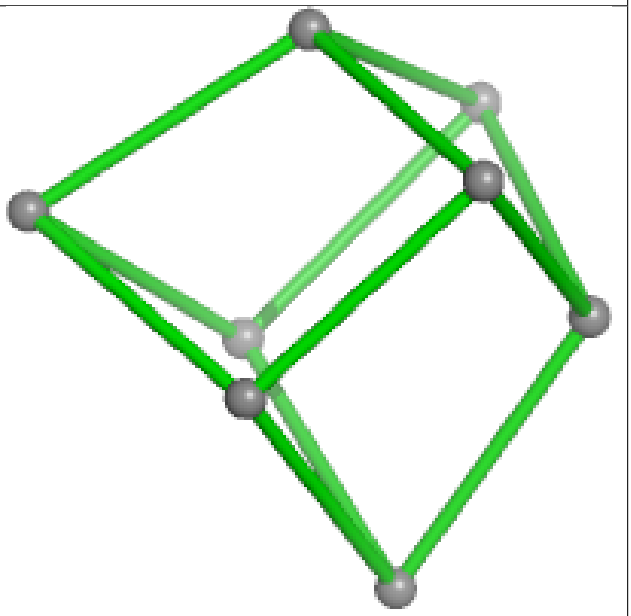
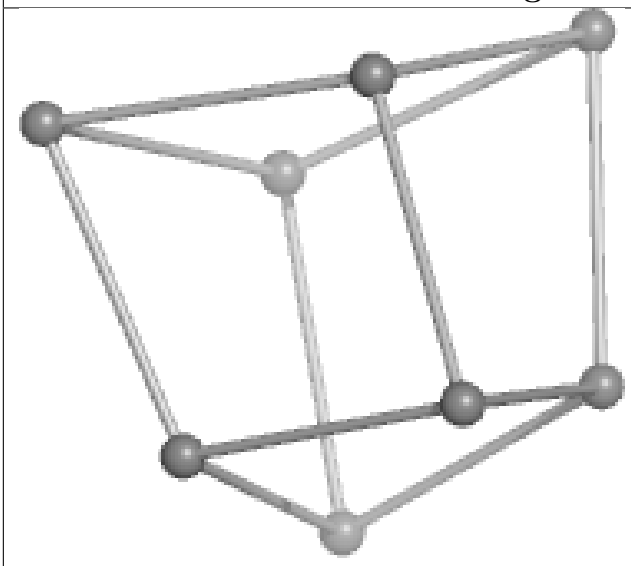


Rings

Ligand SF4 F 1208



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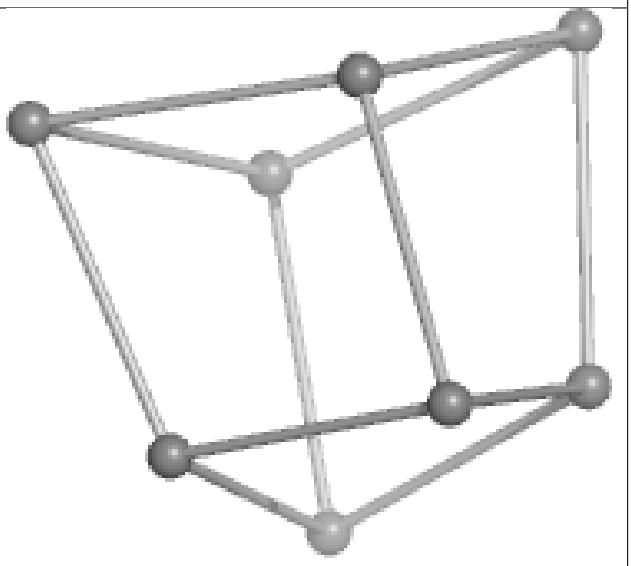
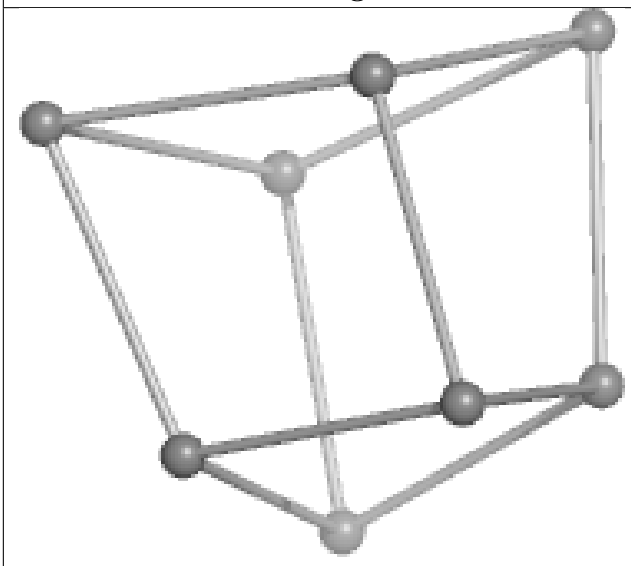


Bond angles



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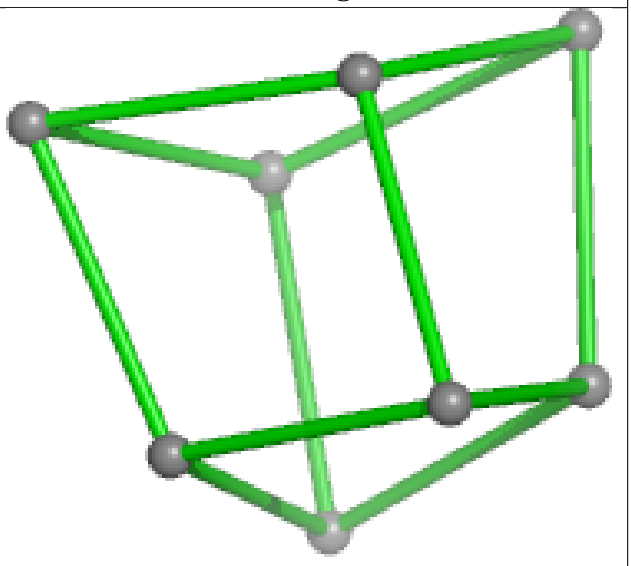
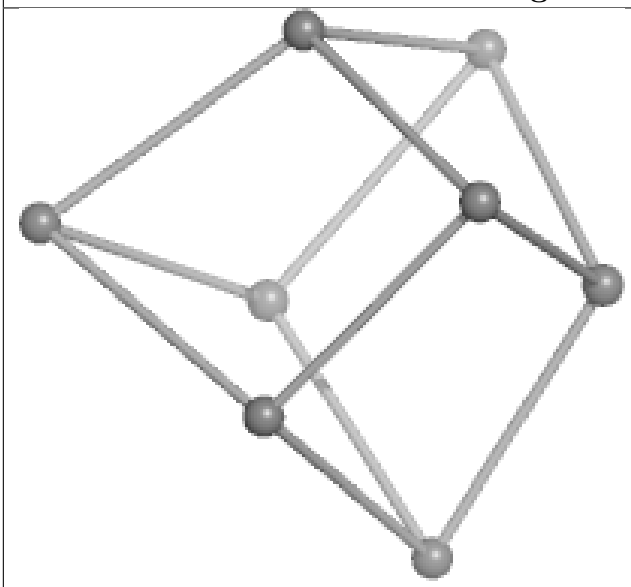


Rings

Ligand SF4 K 605



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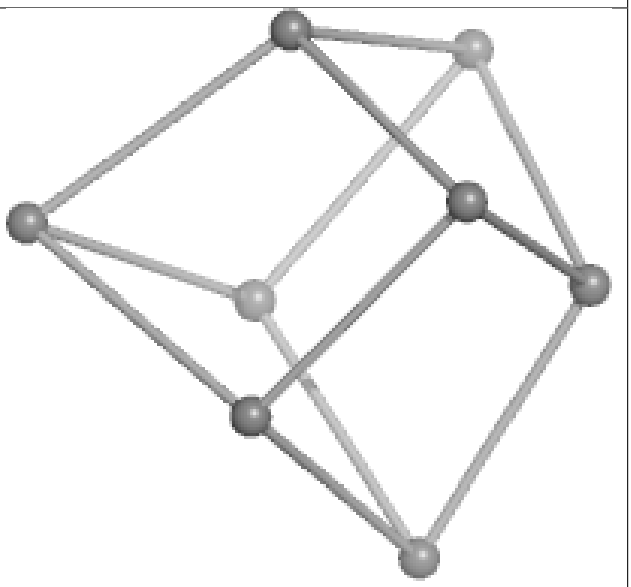
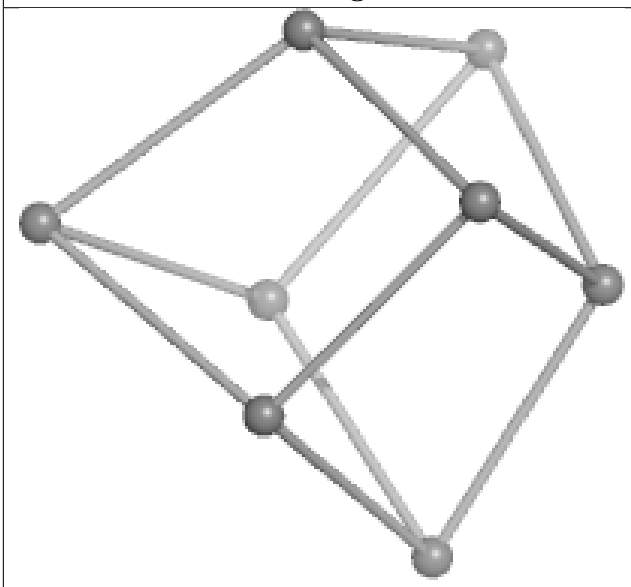


Bond angles



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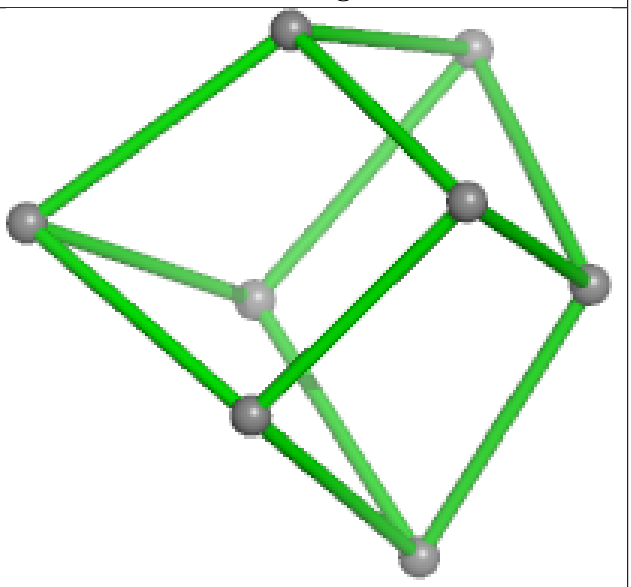
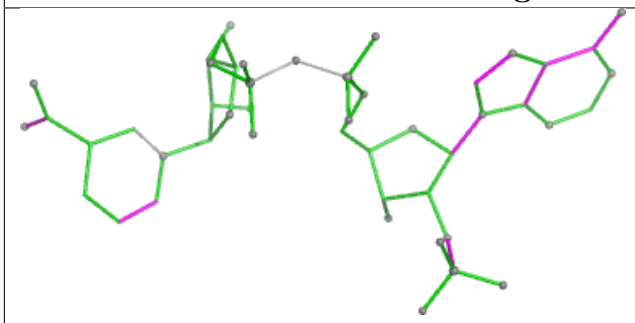


Rings

Ligand NDP C 1203



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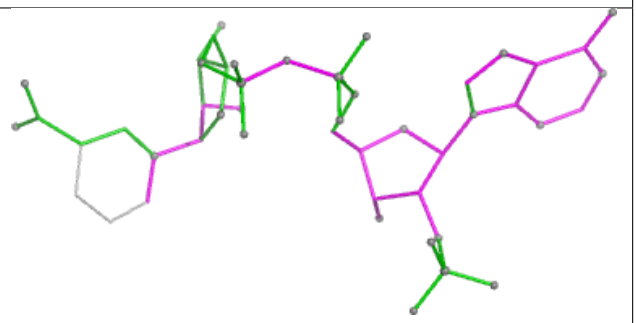
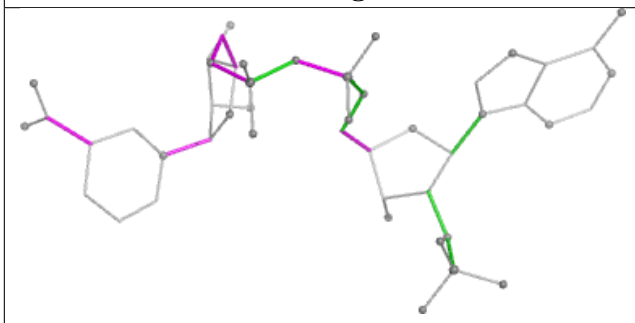


Bond angles



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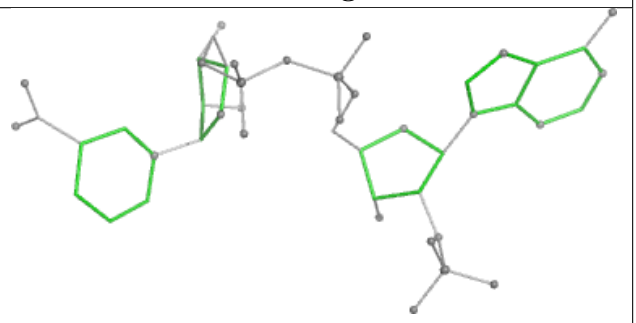
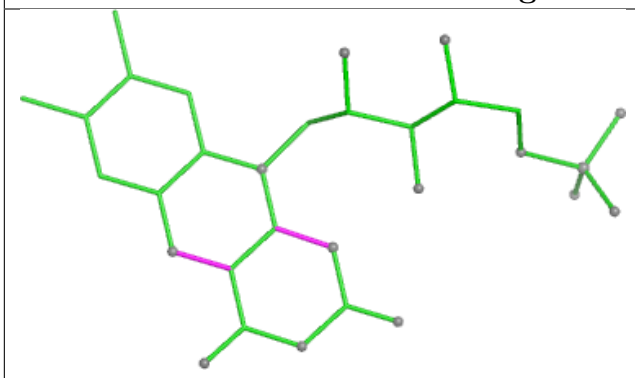
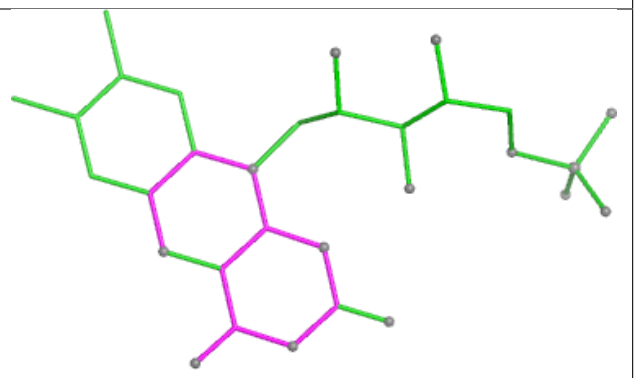


Rings

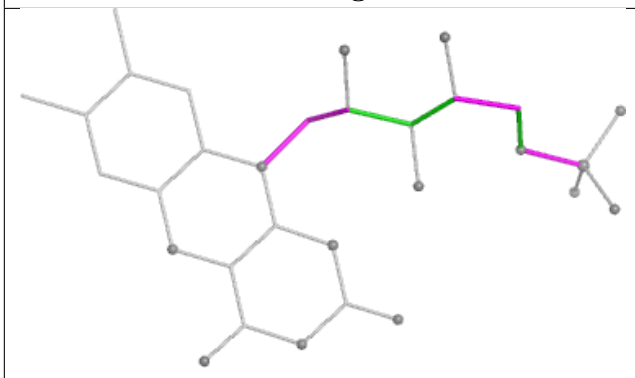
Ligand FMN K 603



Bond lengths



Bond angles



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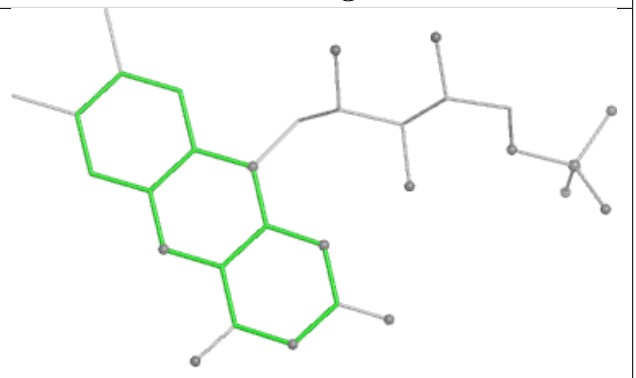
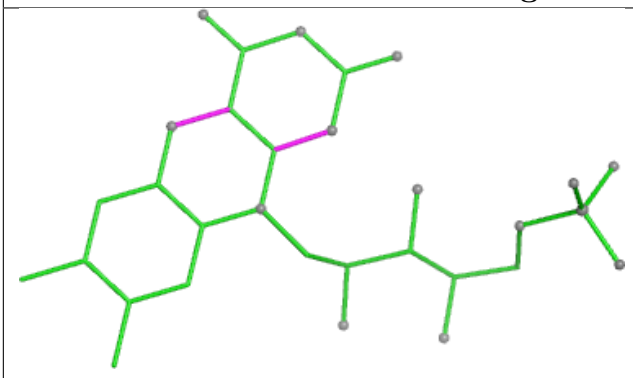


Rings

Ligand FMN E 603



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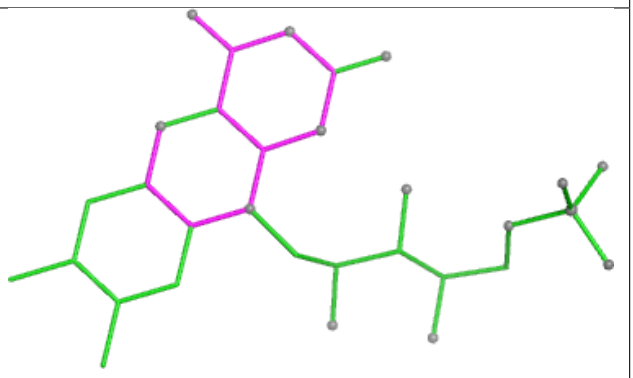
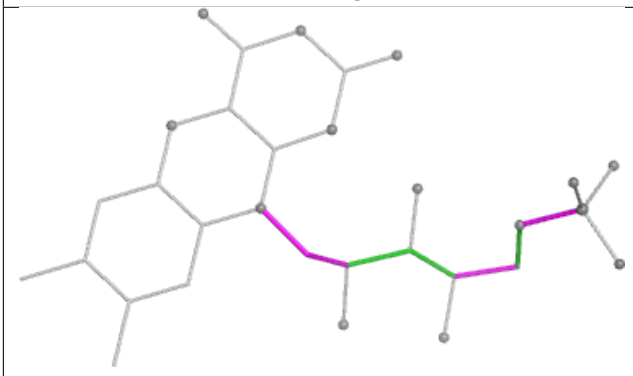
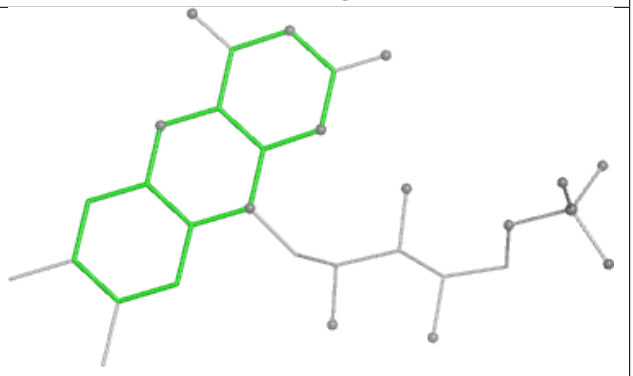


Bond angles

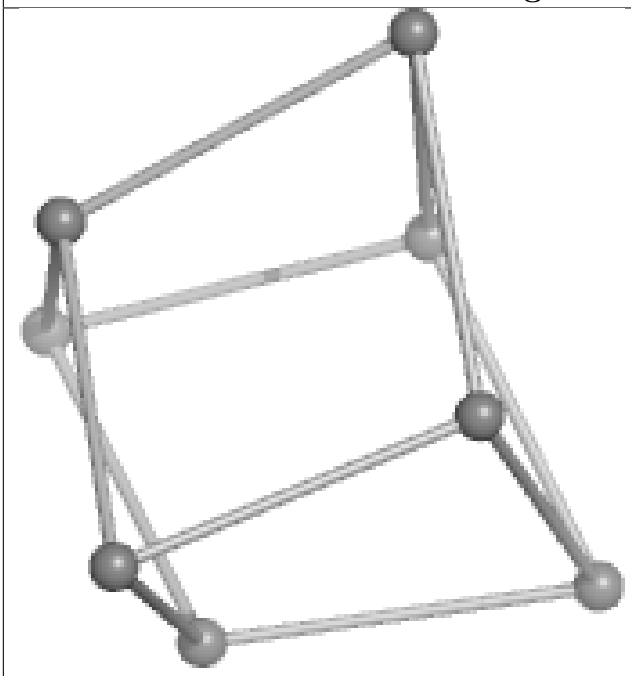


Torsions



Rings

Ligand SF4 F 1204



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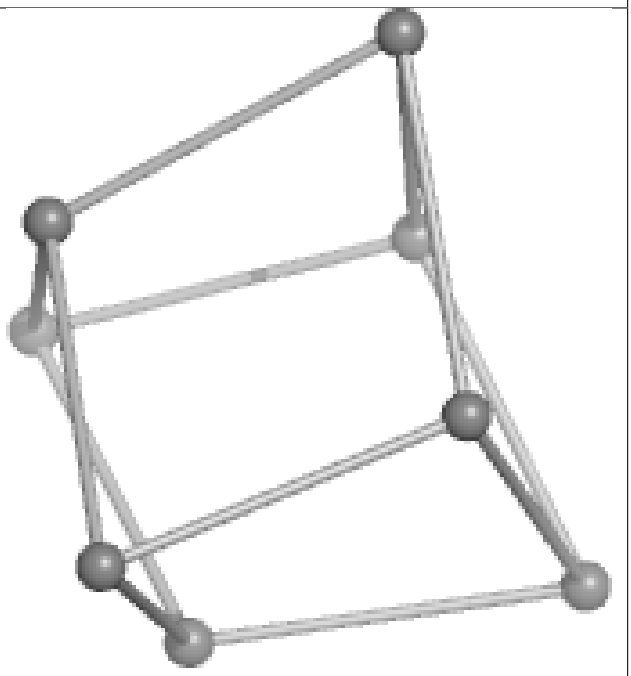
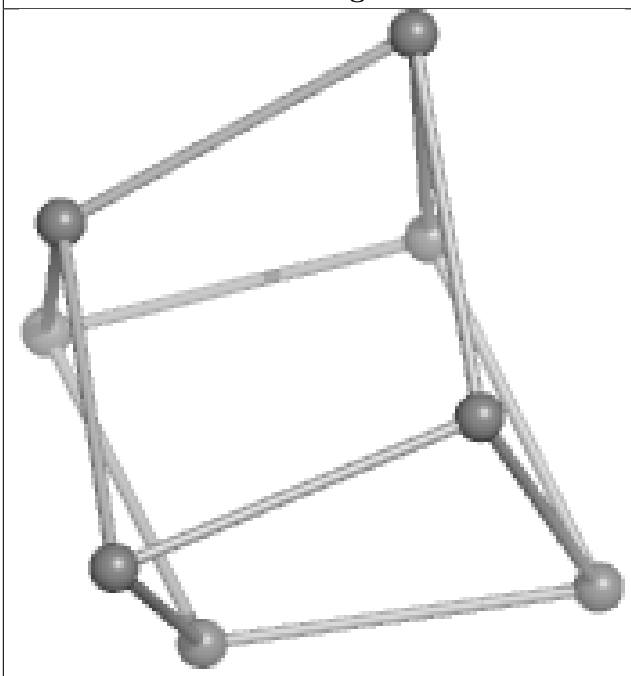


Bond angles



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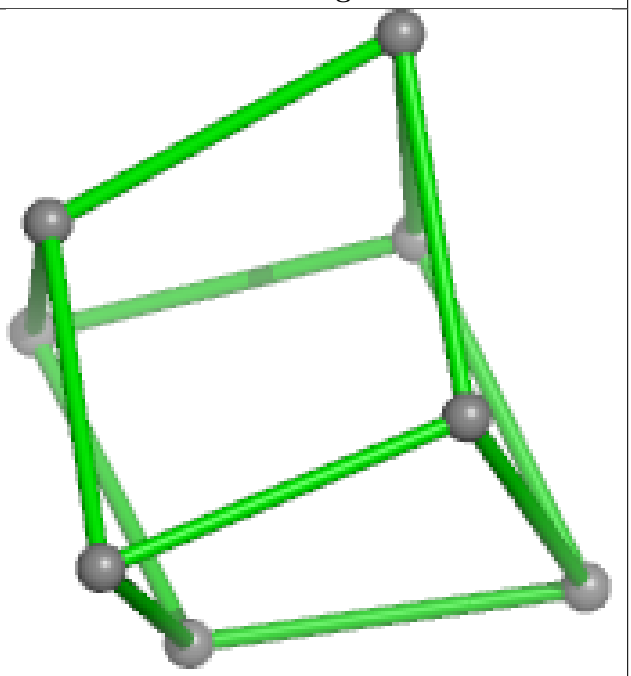
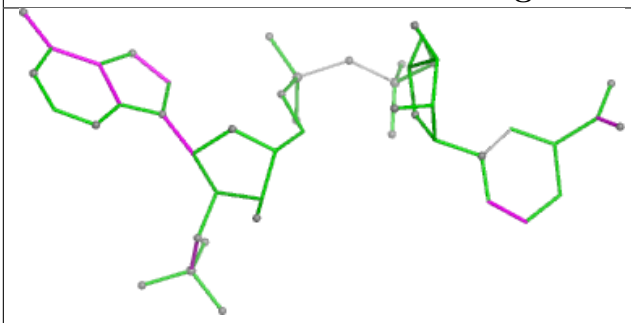


Rings

Ligand NDP L 1203



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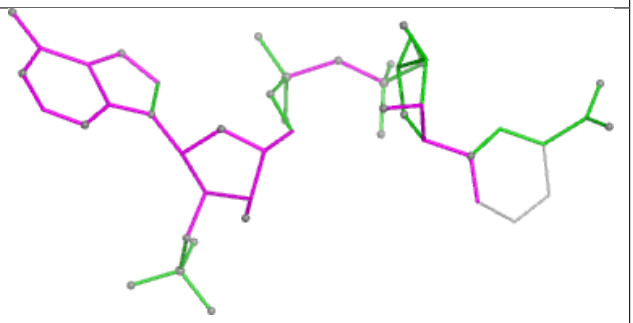

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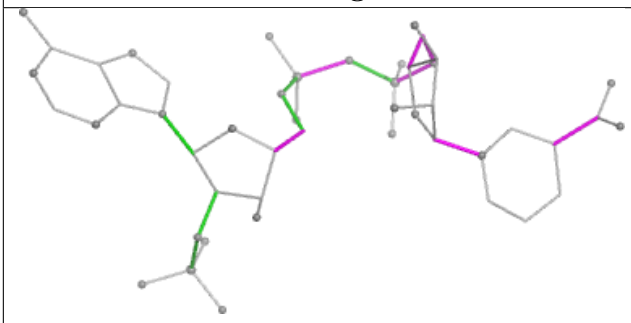

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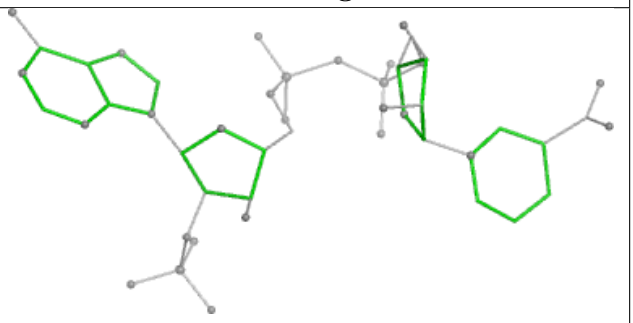
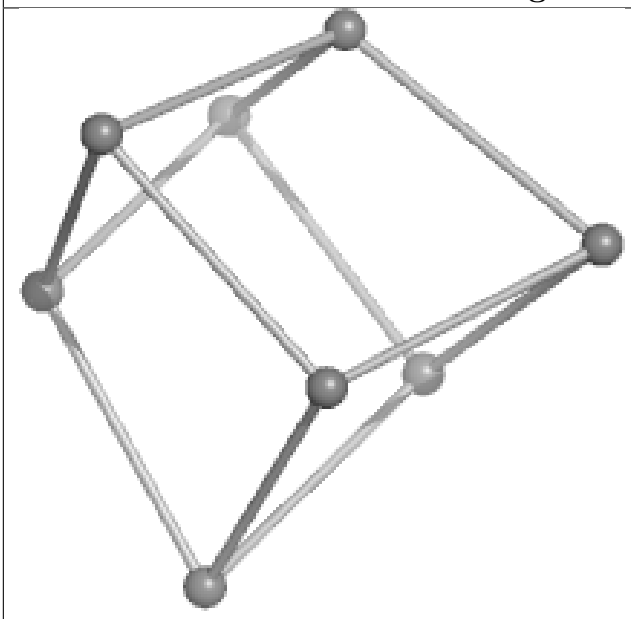


Rings

Ligand SF4 I 1205



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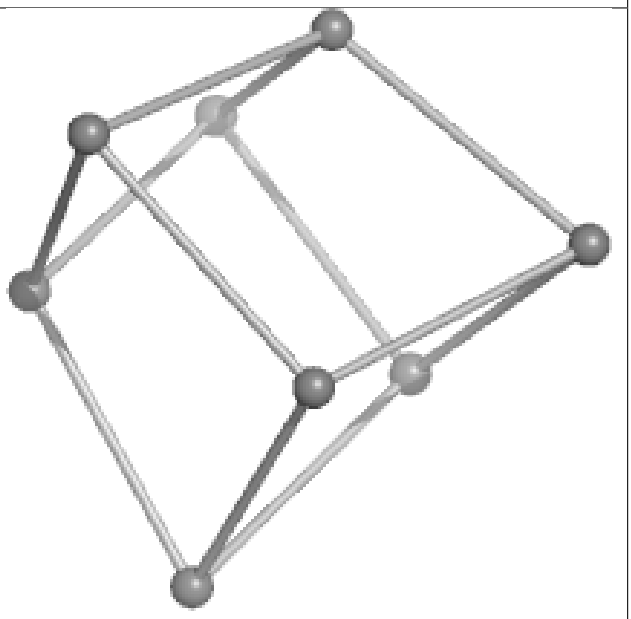

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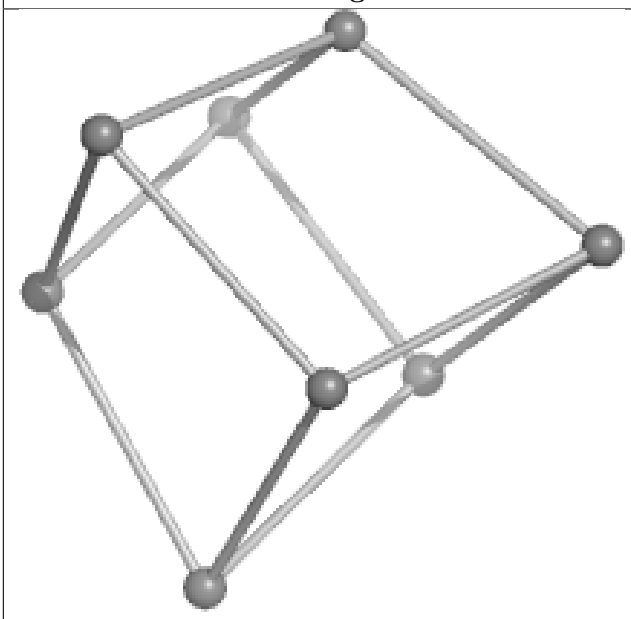

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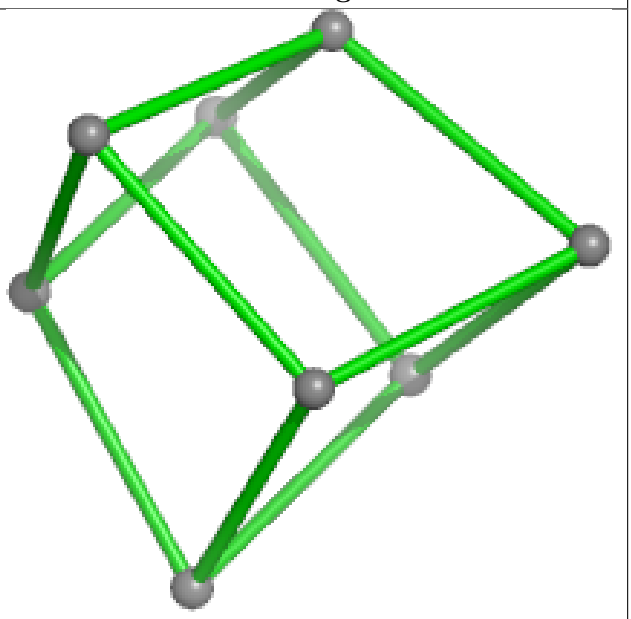
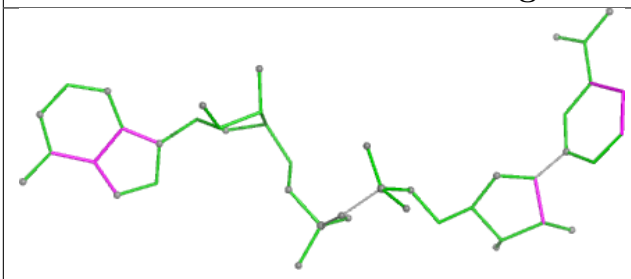


Rings

Ligand NAD H 606



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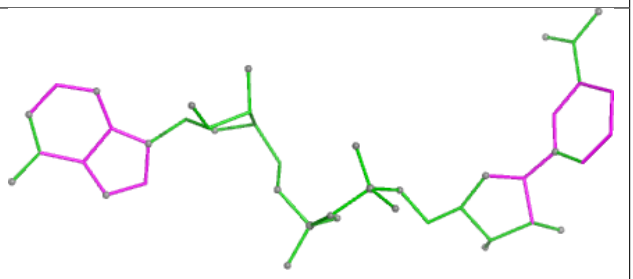

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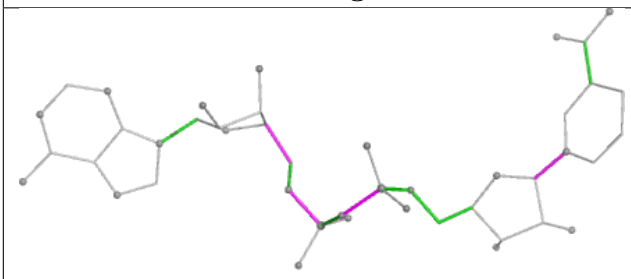

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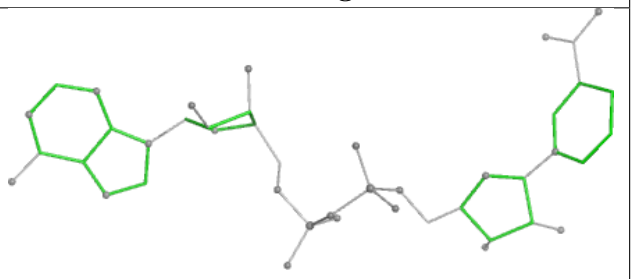
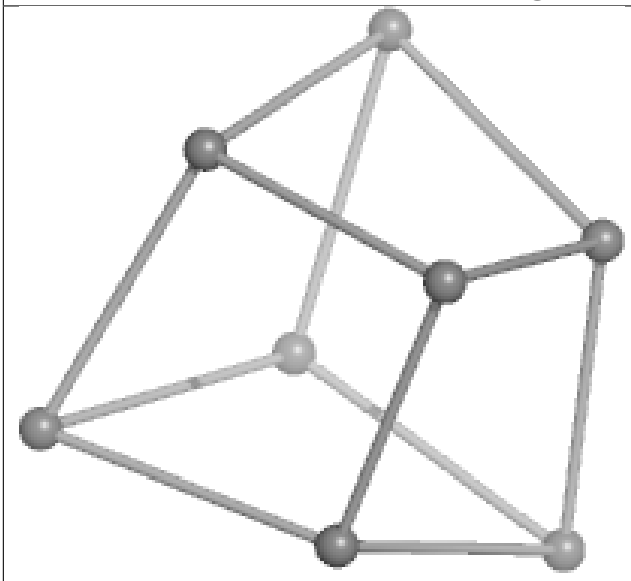


Rings

Ligand SF4 I 1206



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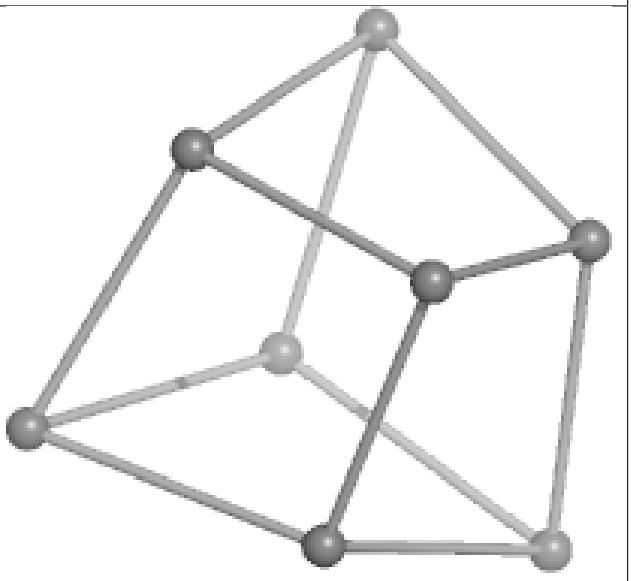

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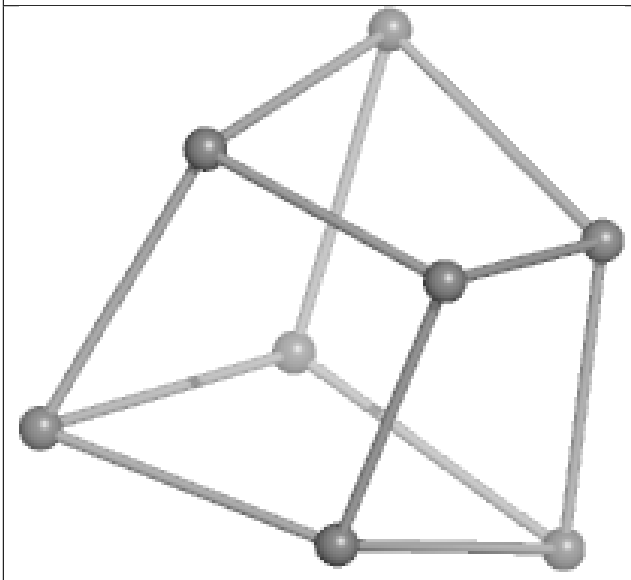

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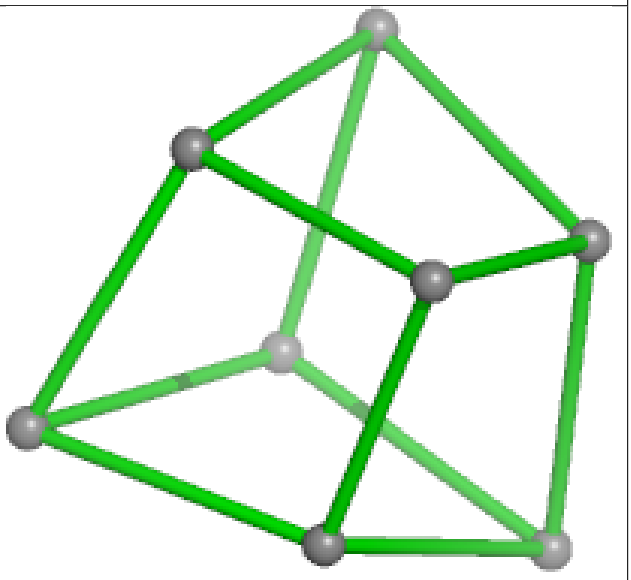
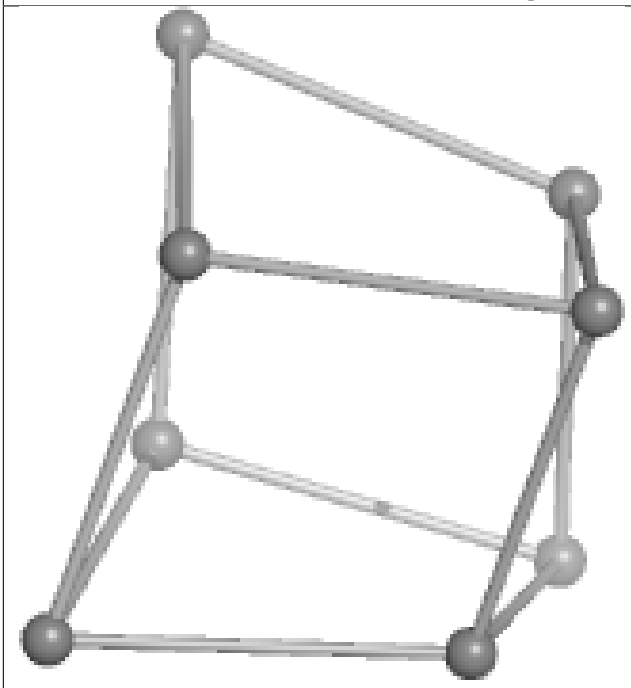


Rings

Ligand SF4 C 1204



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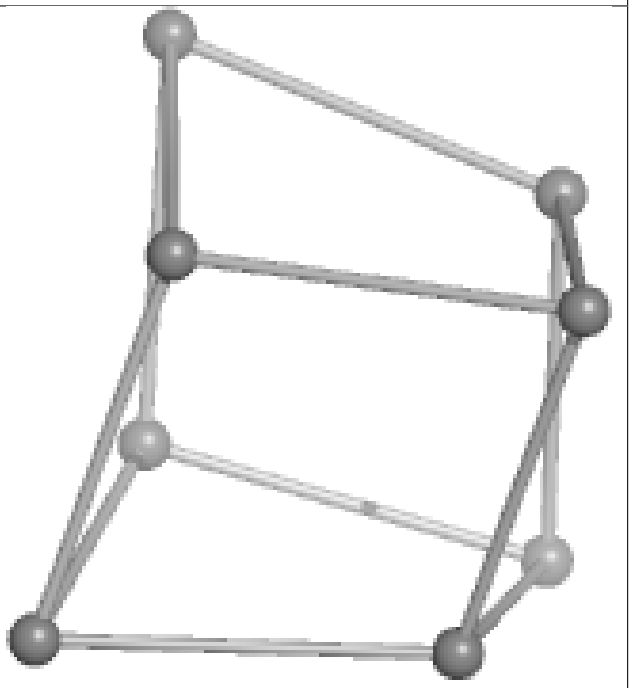

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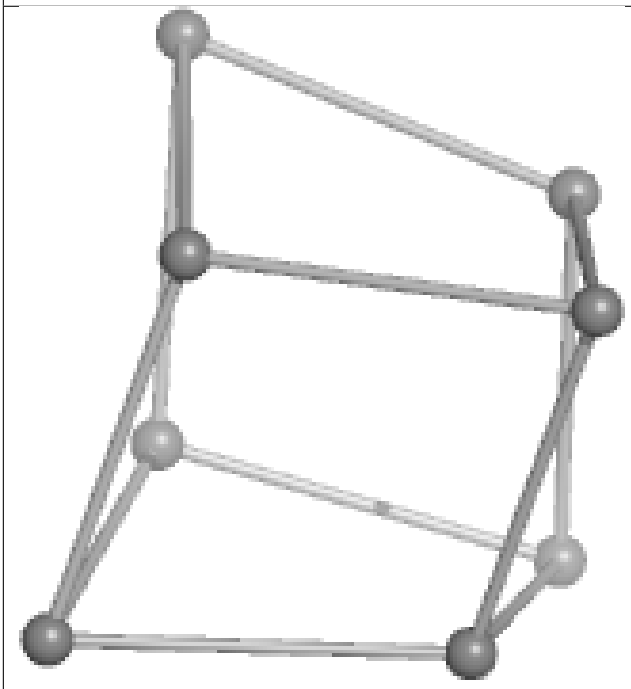

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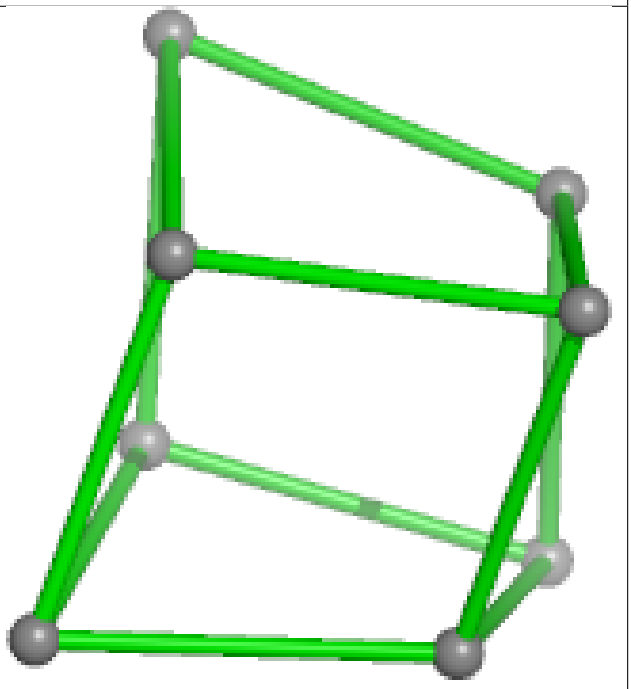
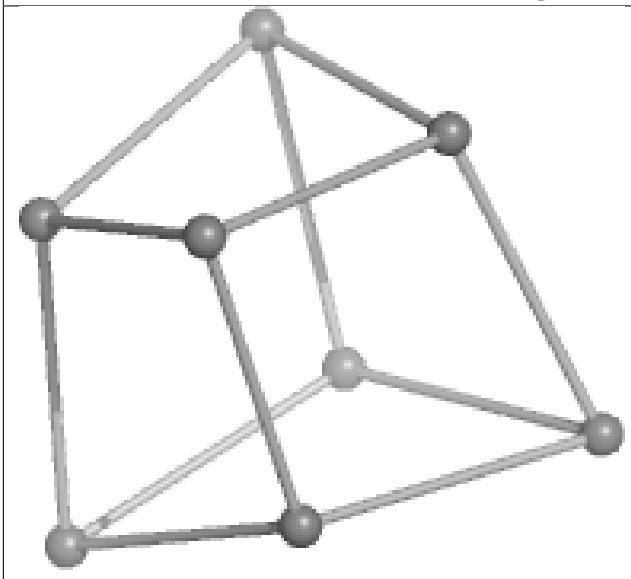


Rings

Ligand SF4 E 604



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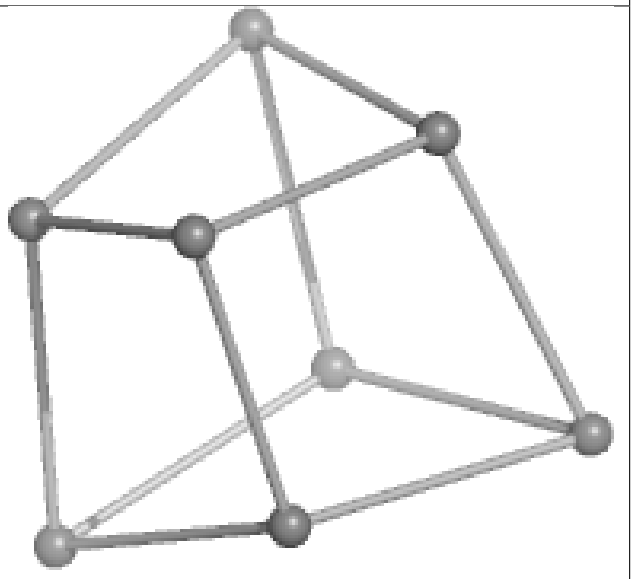

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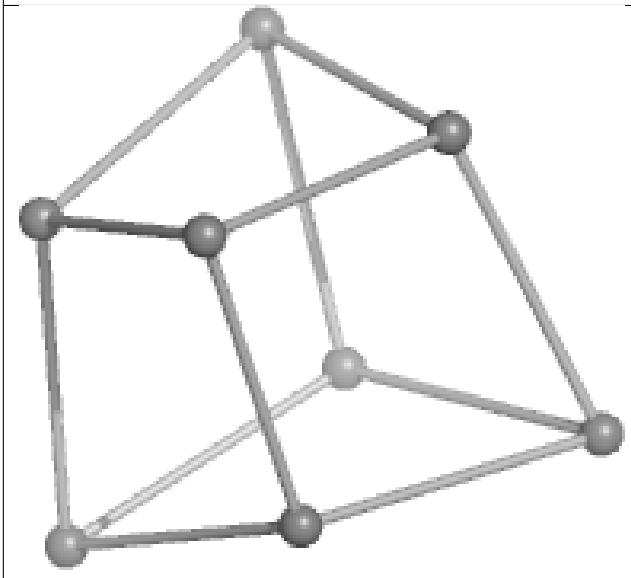

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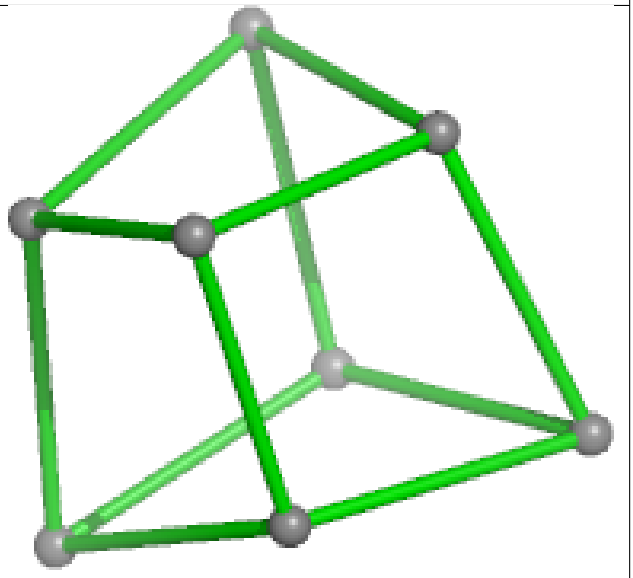
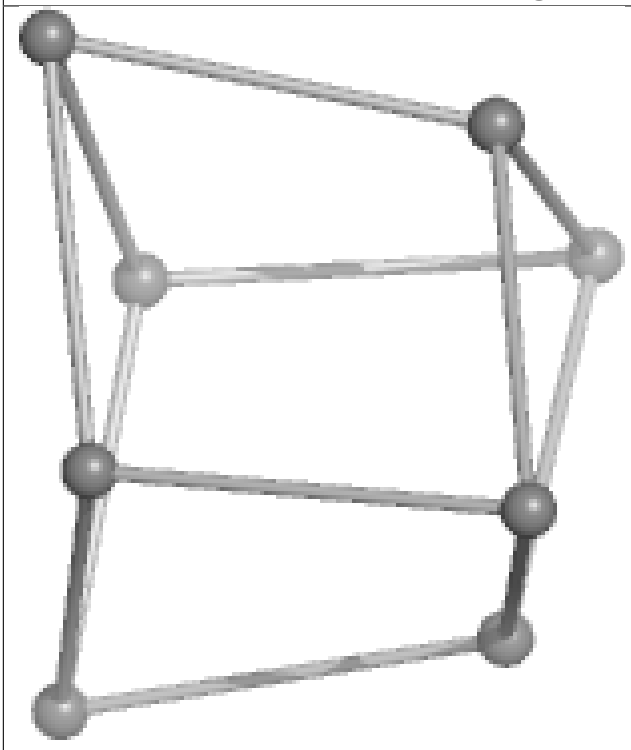


Rings

Ligand SF4 H 607



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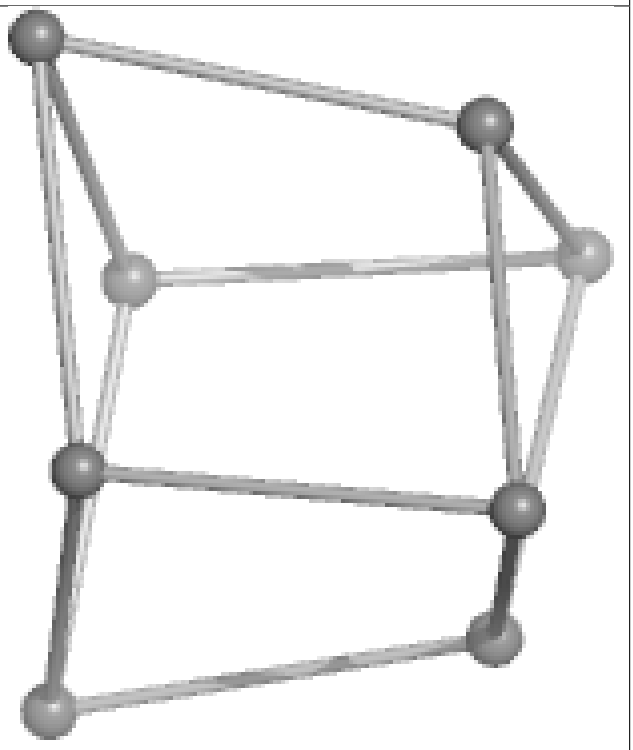

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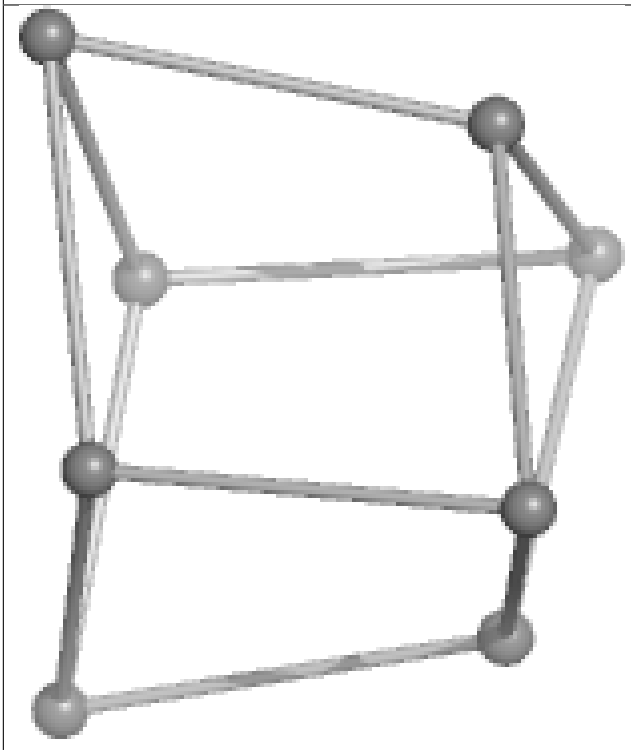

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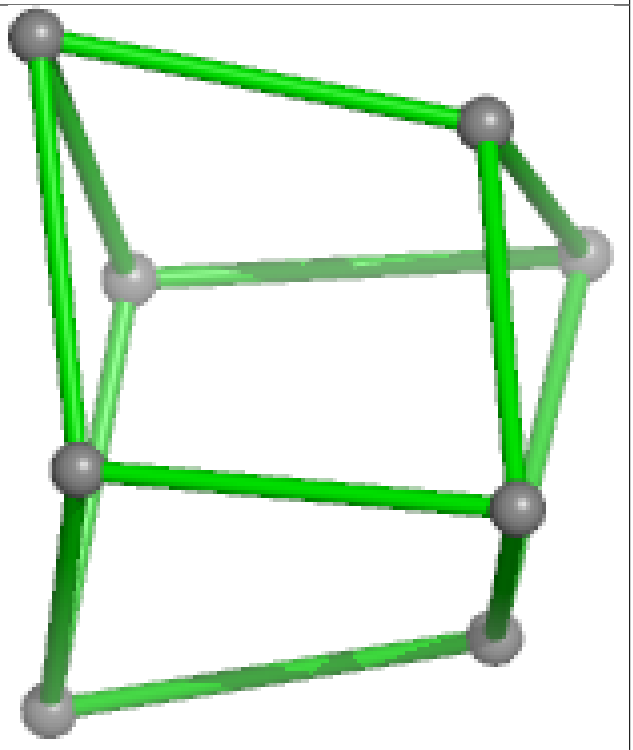
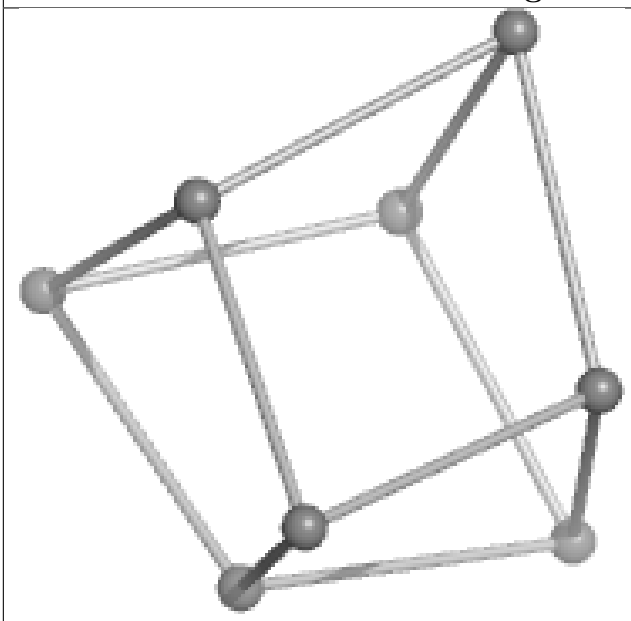


Rings

Ligand SF4 L 1202



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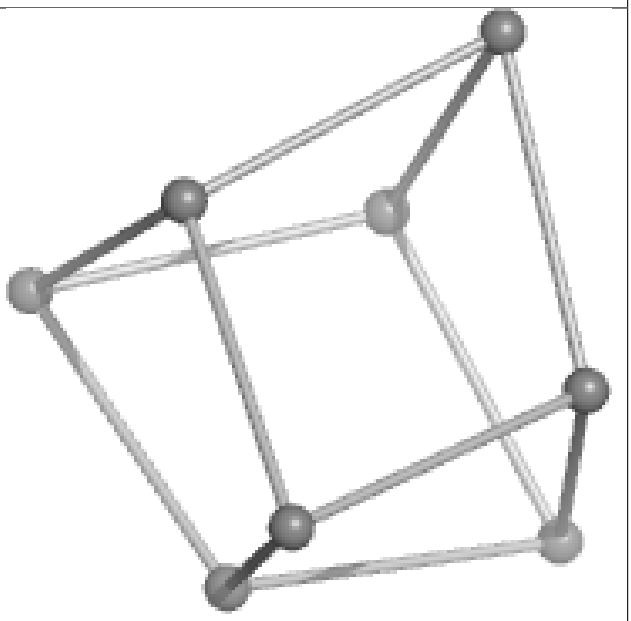

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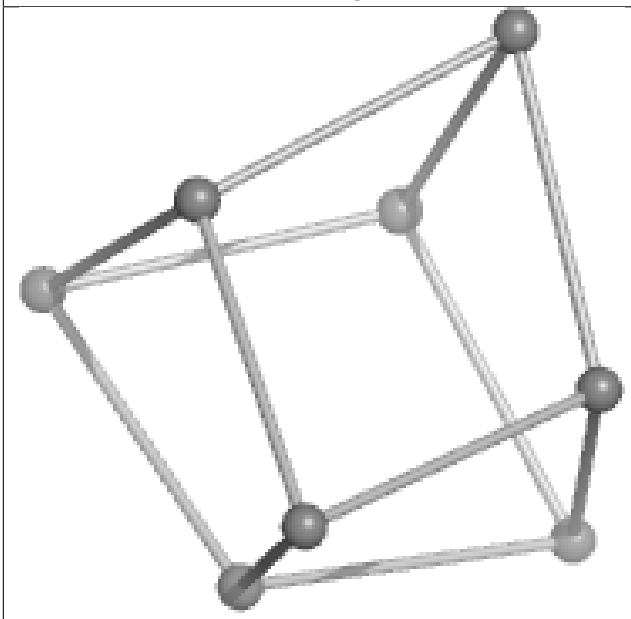

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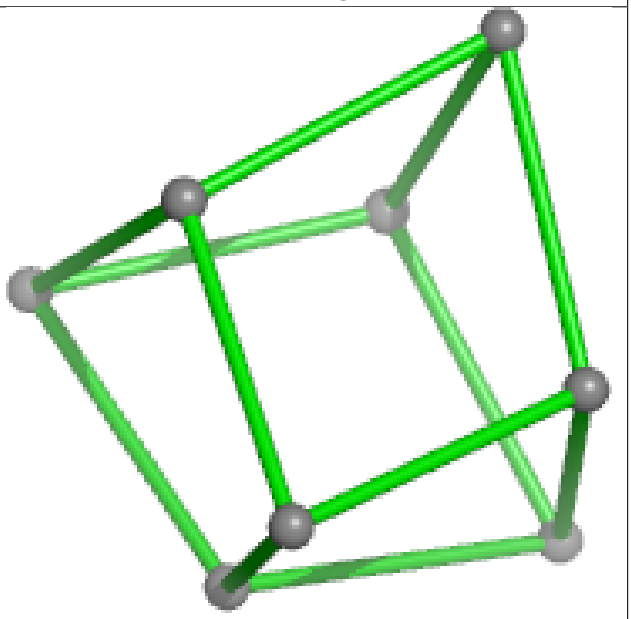
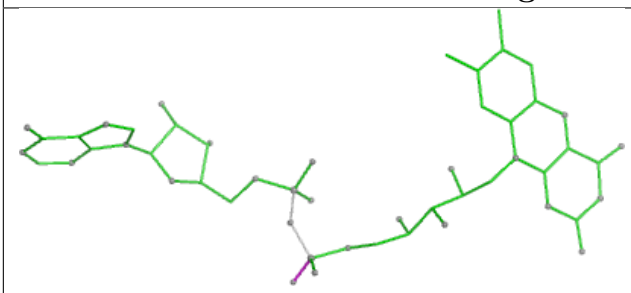


Rings

Ligand FAD L 1201



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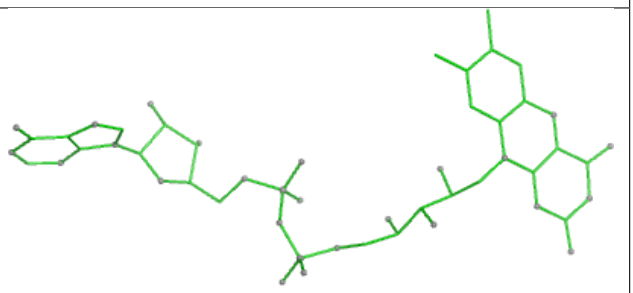

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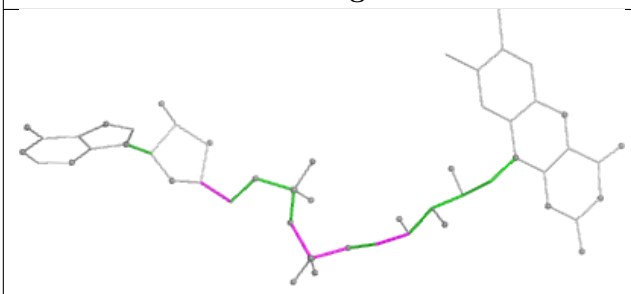

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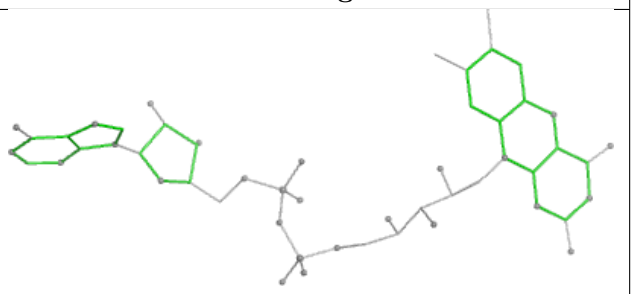
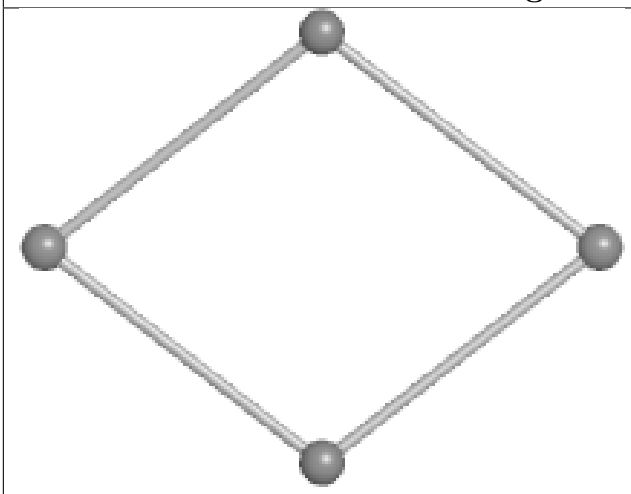


Rings

Ligand FES I 1209



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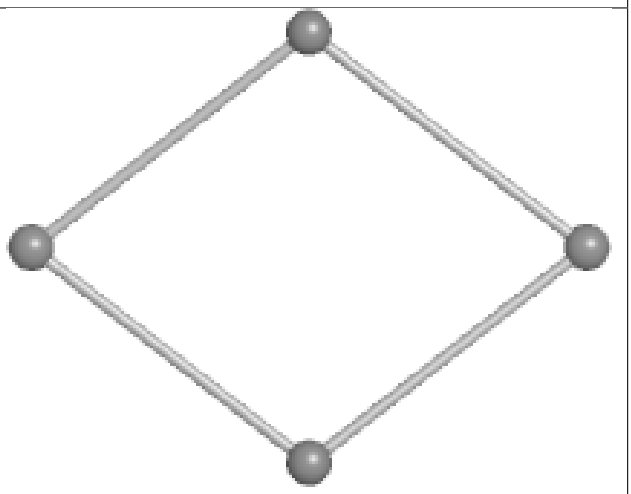

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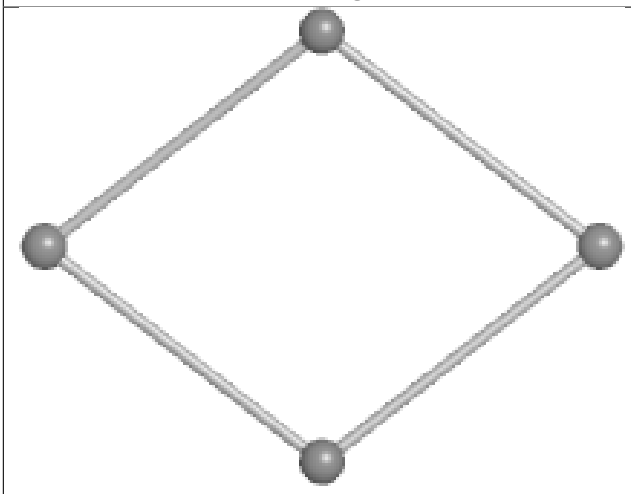

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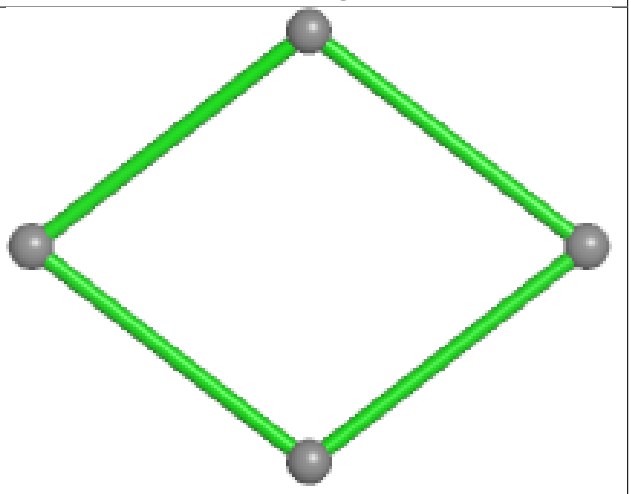
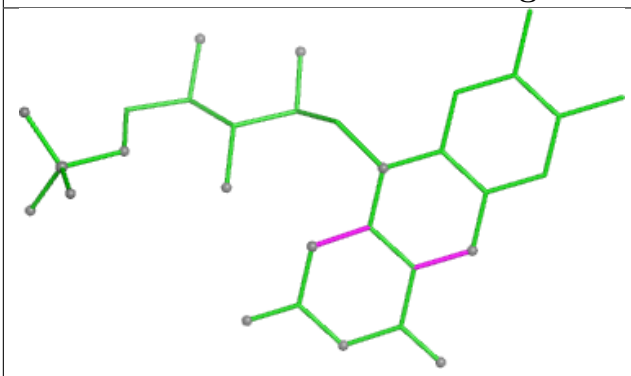


Rings

Ligand FMN B 603



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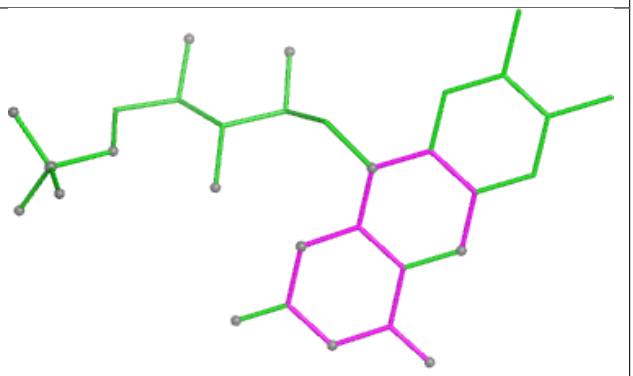

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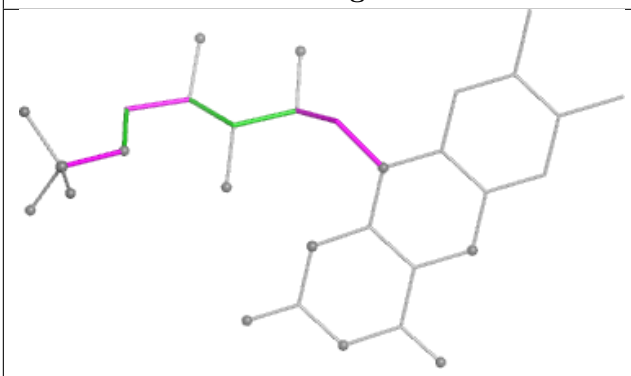

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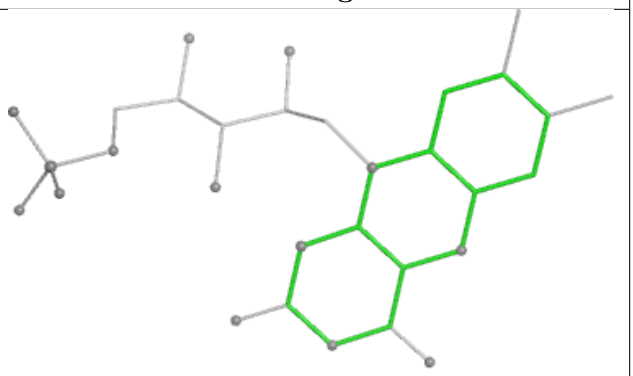
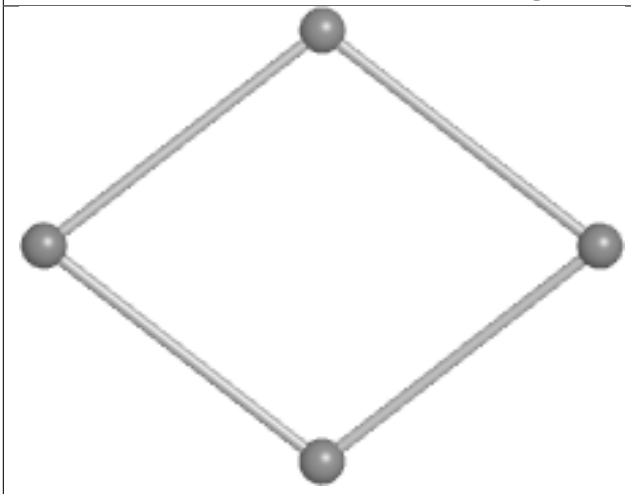


Rings

Ligand FES A 201



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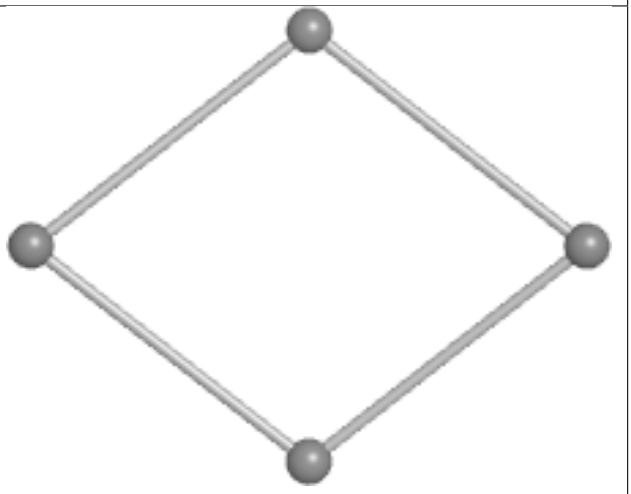
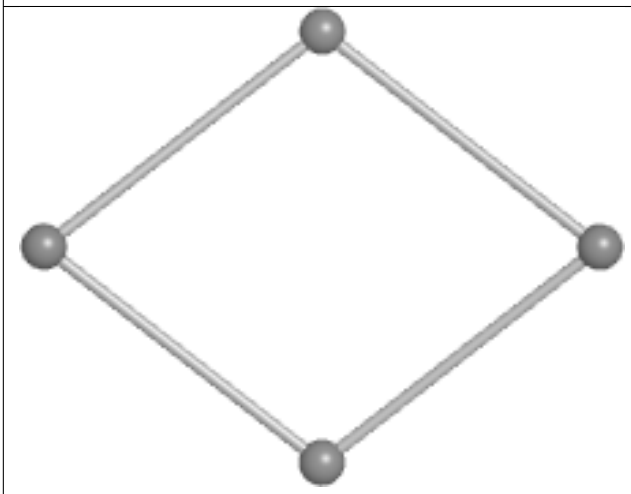


Bond angles



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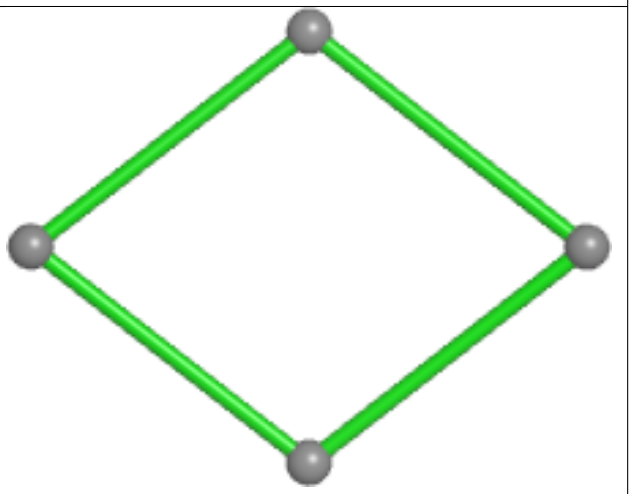
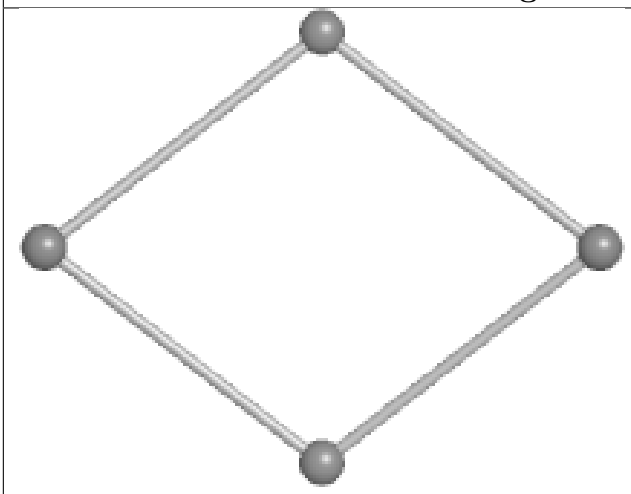


Rings

Ligand FES C 1209



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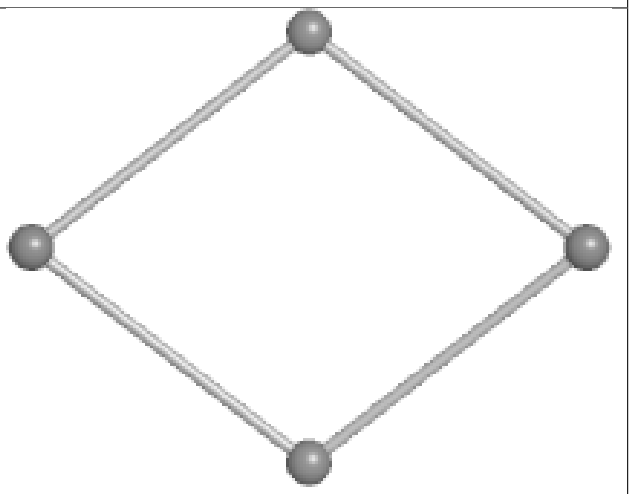
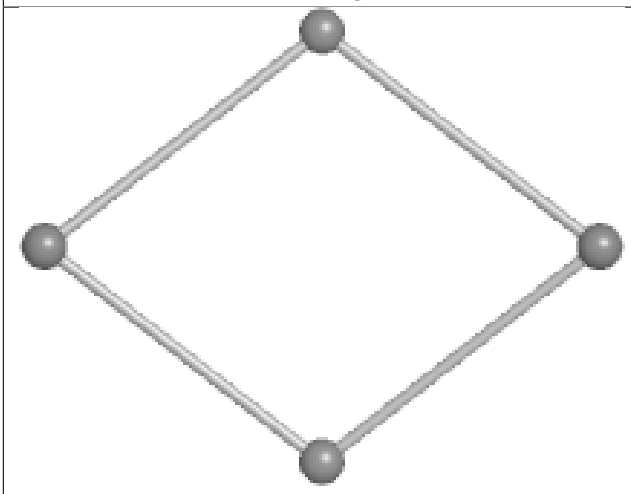


Bond angles



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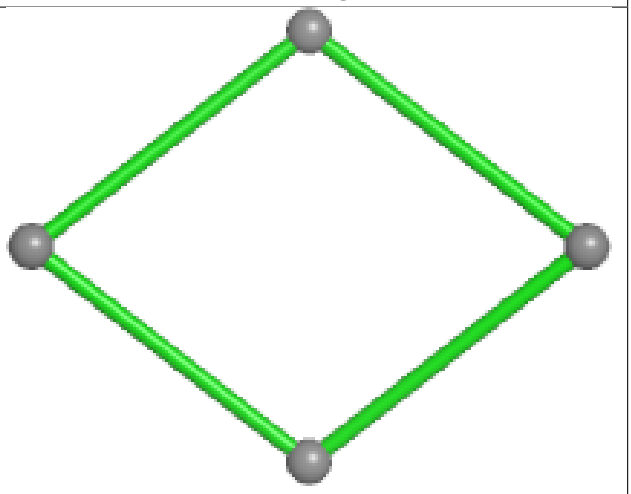
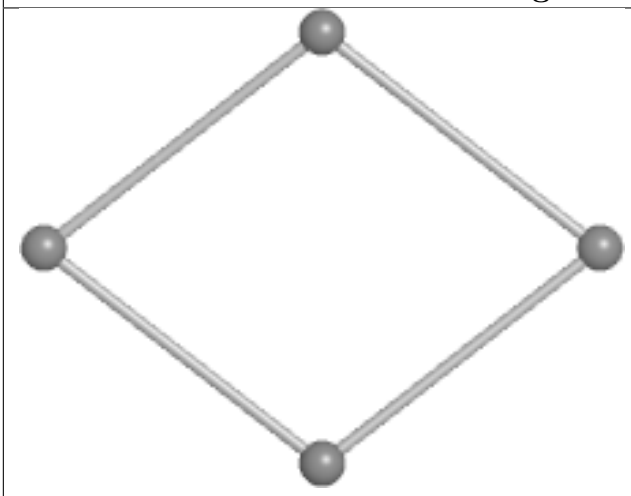
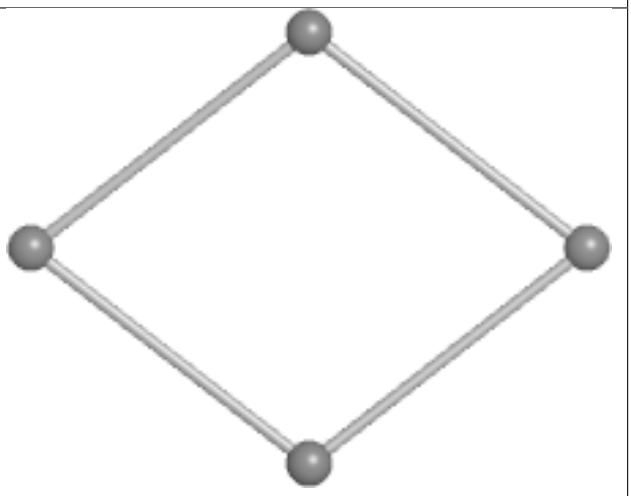


Rings

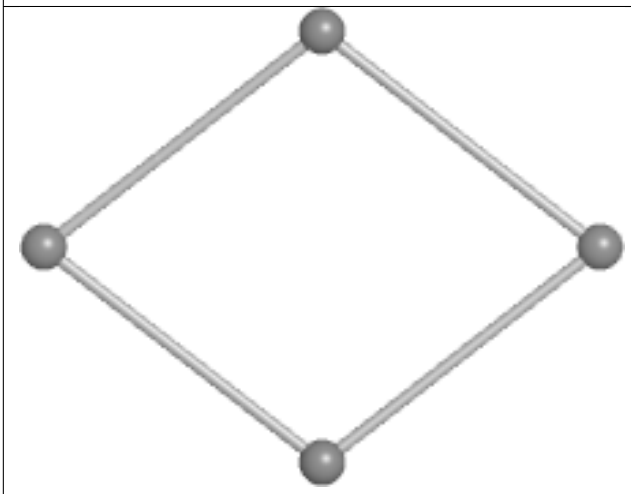
Ligand FES J 201



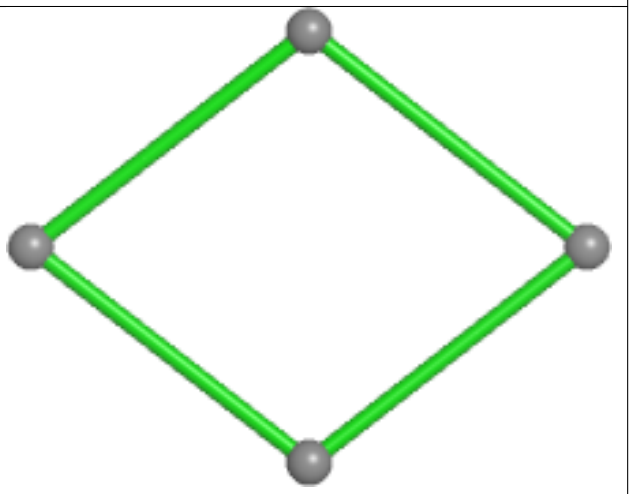
Bond lengths



Bond angles

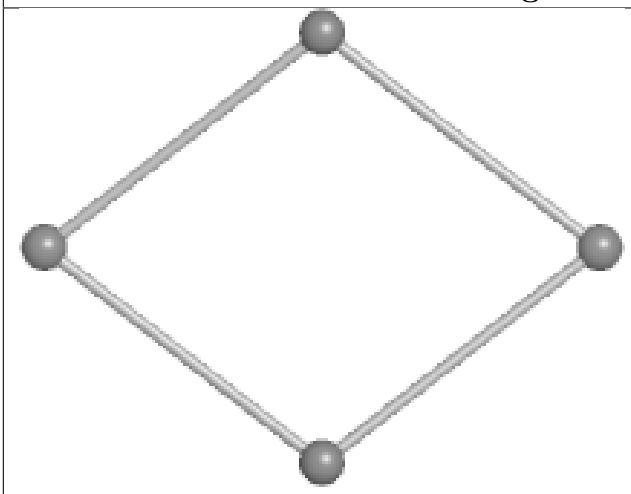


Torsions



Rings

Ligand FES L 1209



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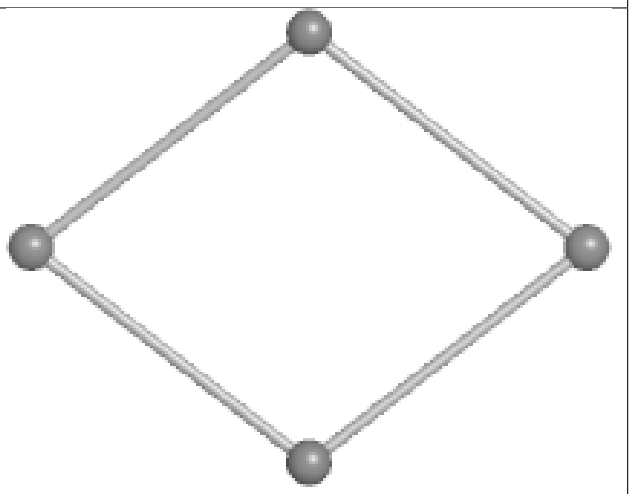

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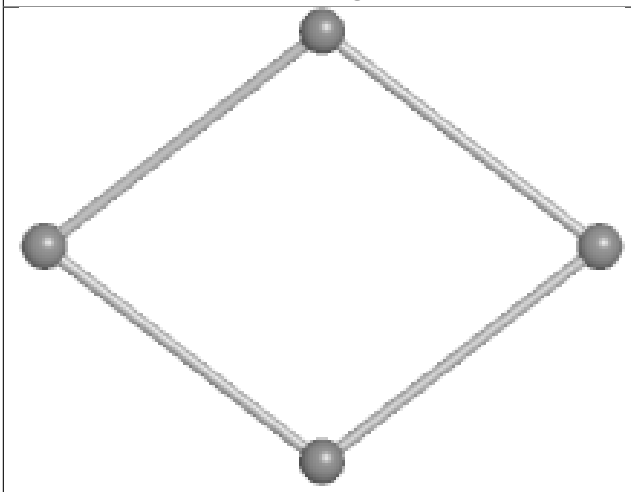

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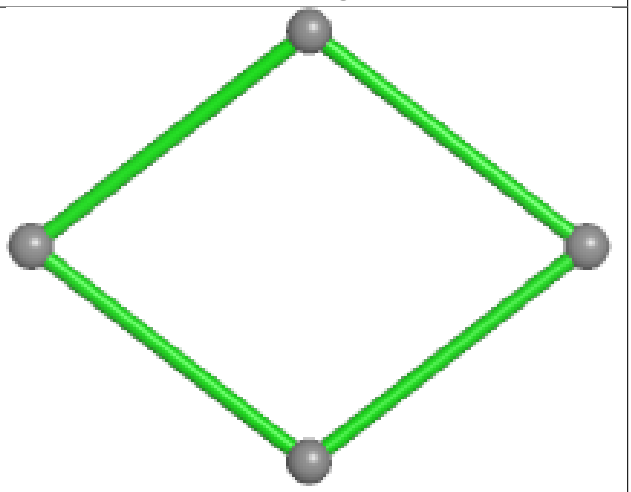
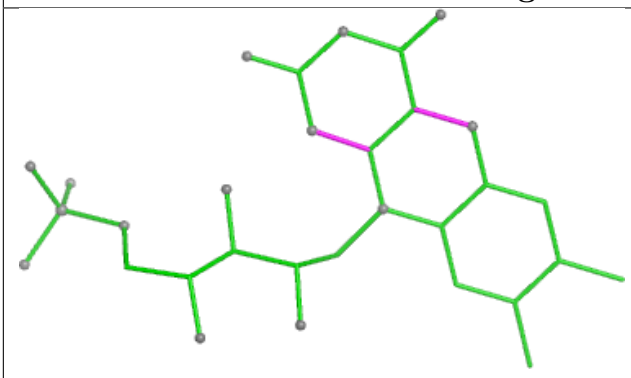


Rings

Ligand FMN H 603



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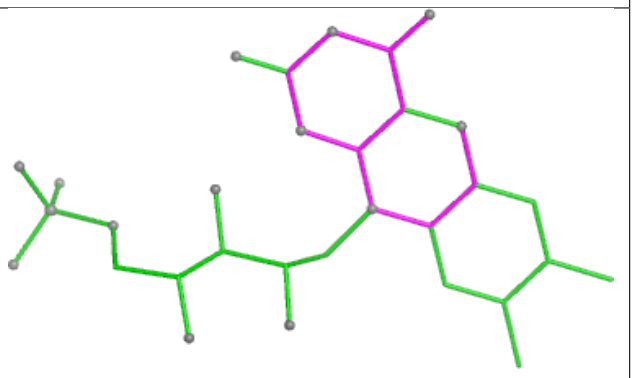

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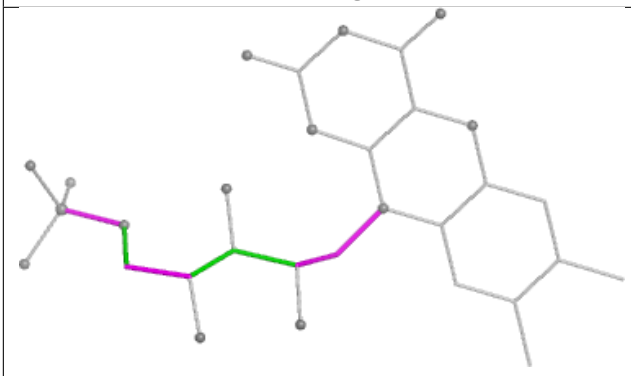

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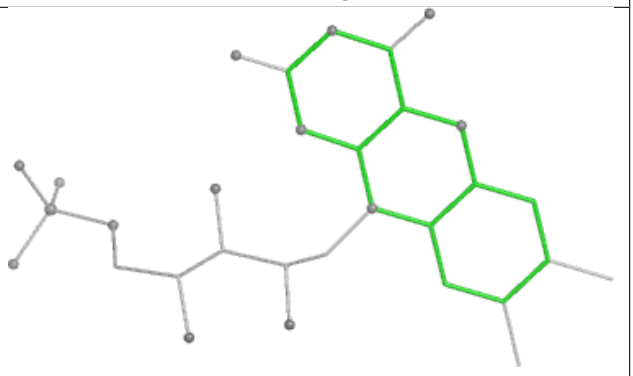
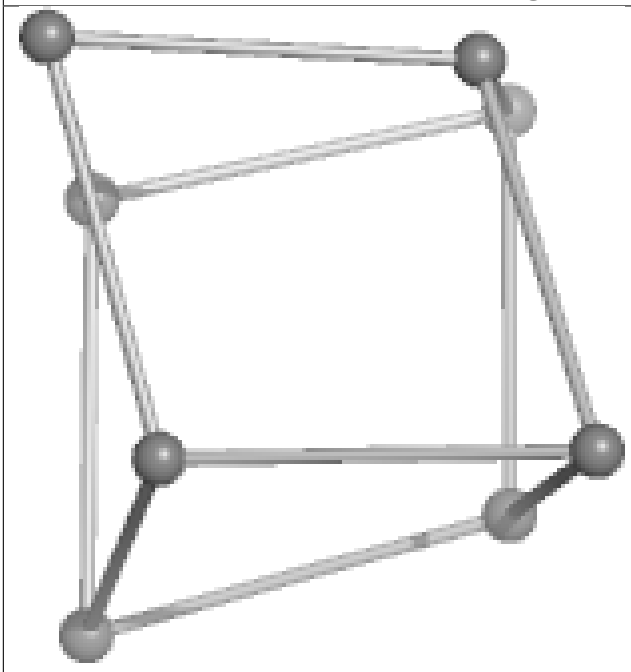


Rings

Ligand SF4 L 1207



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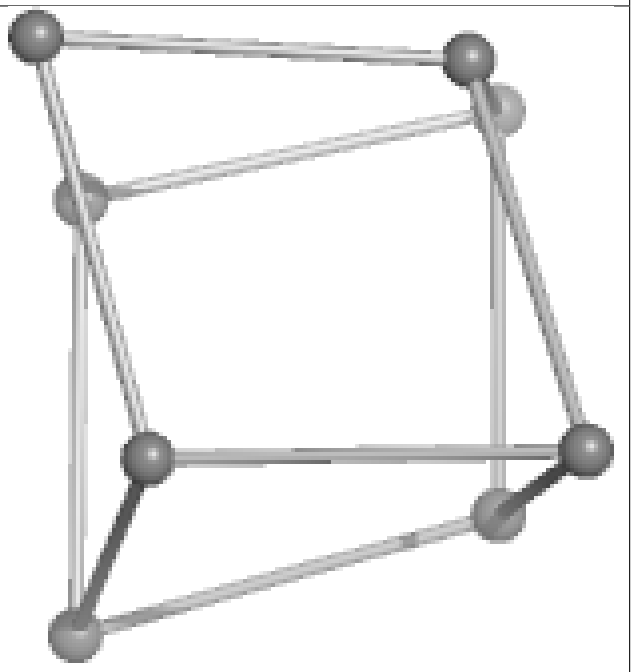
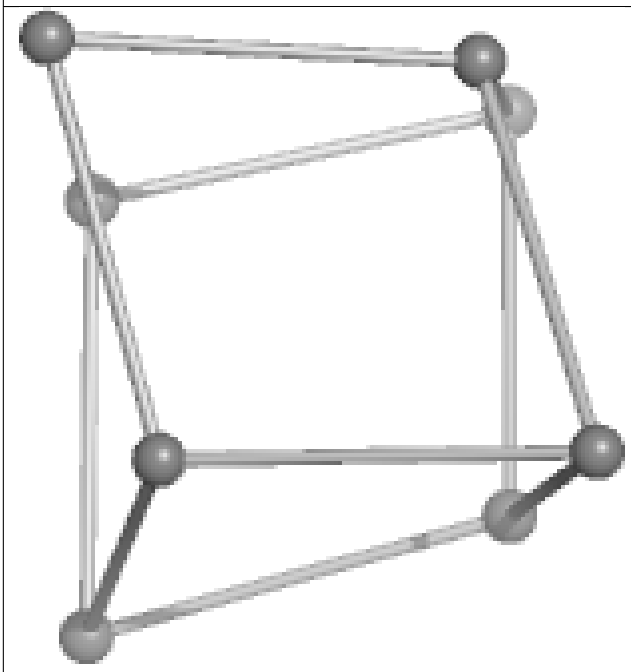


Bond angles



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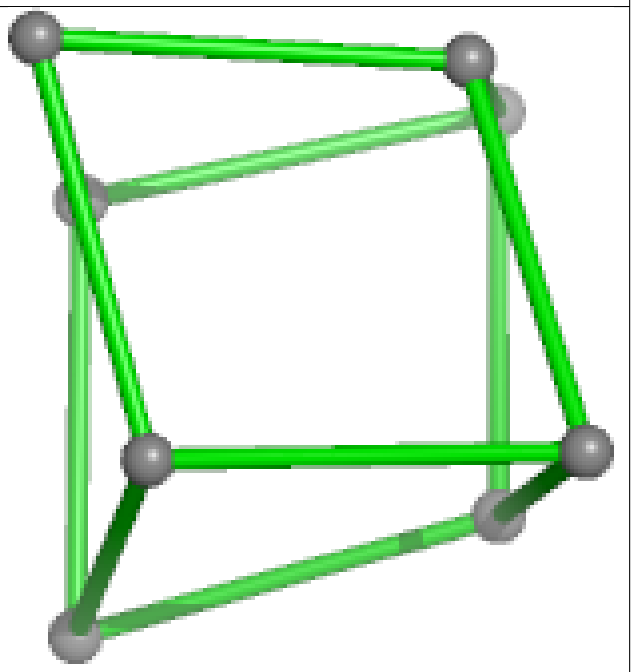
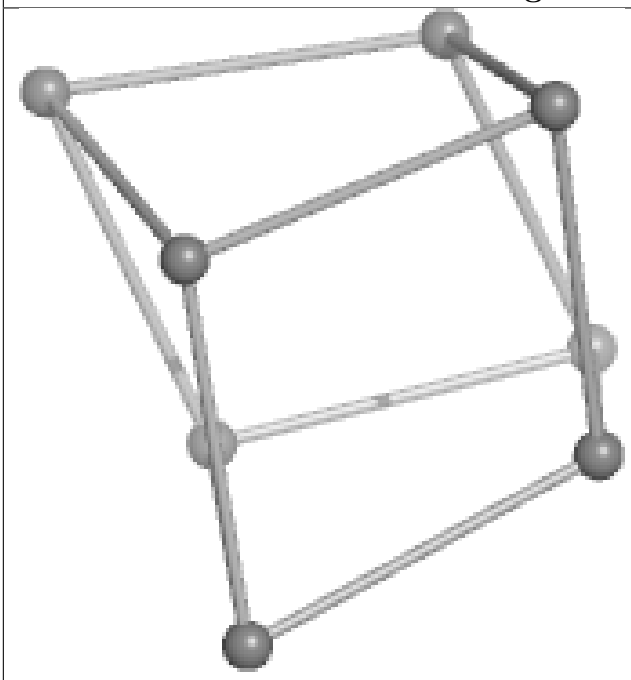


Rings

Ligand SF4 L 1204



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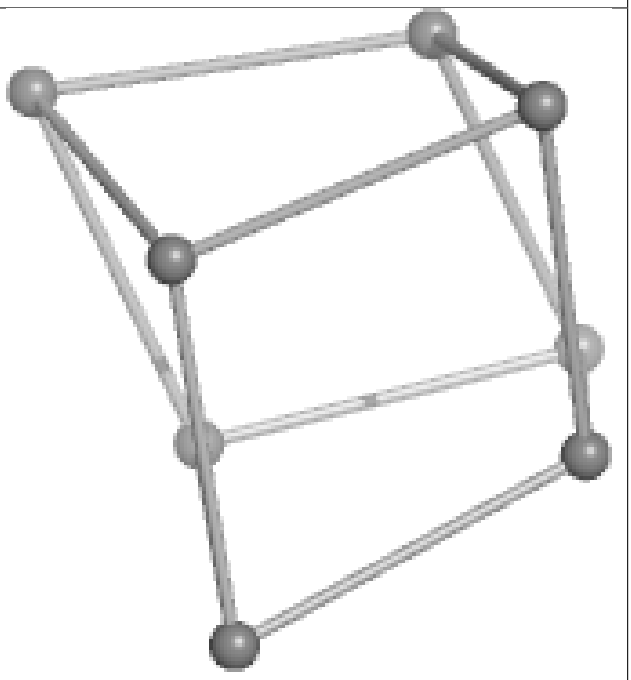

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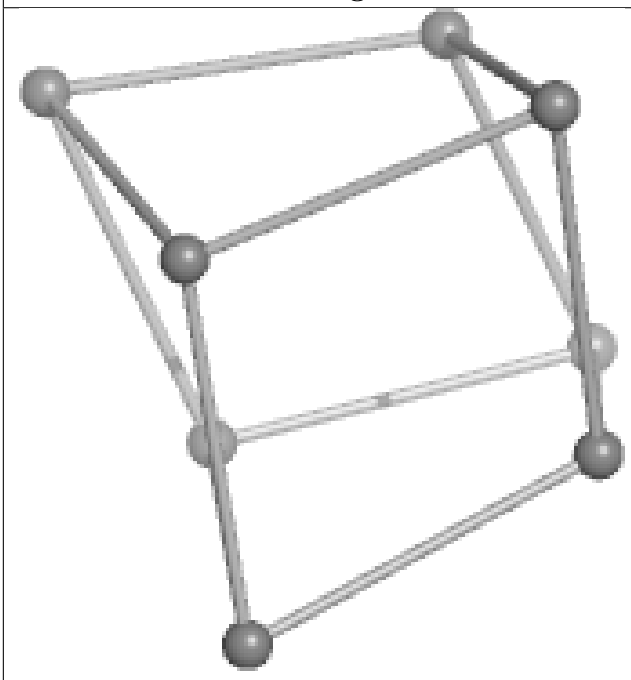

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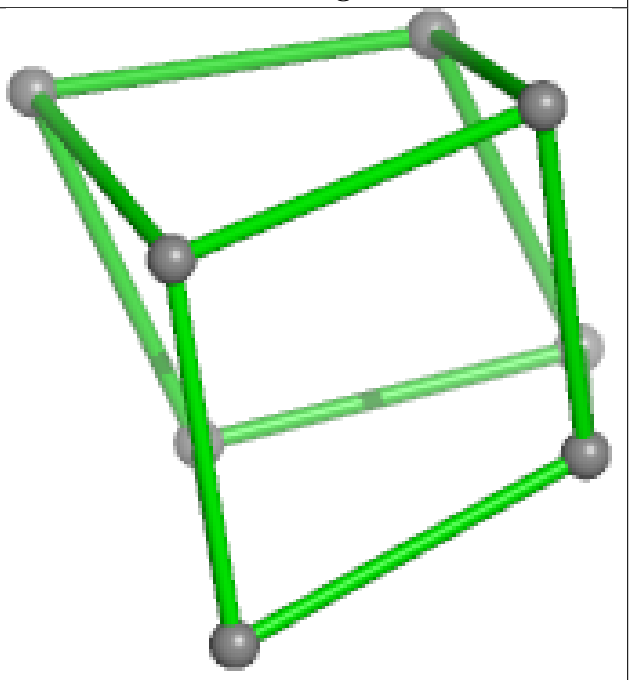
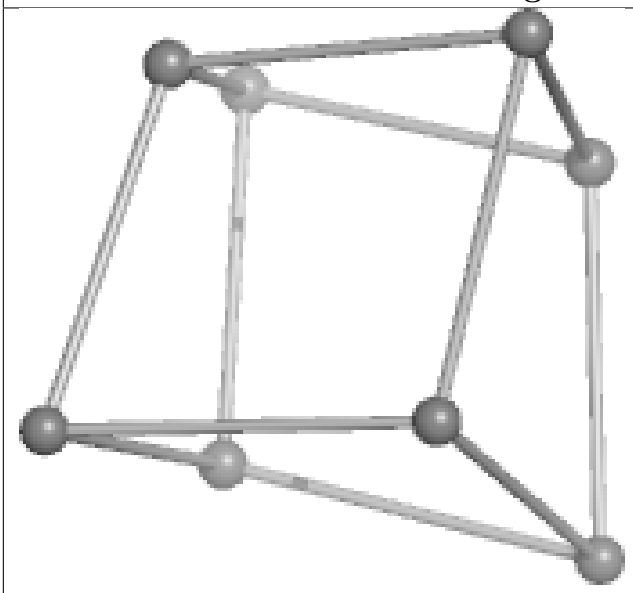


Rings

Ligand SF4 F 1202



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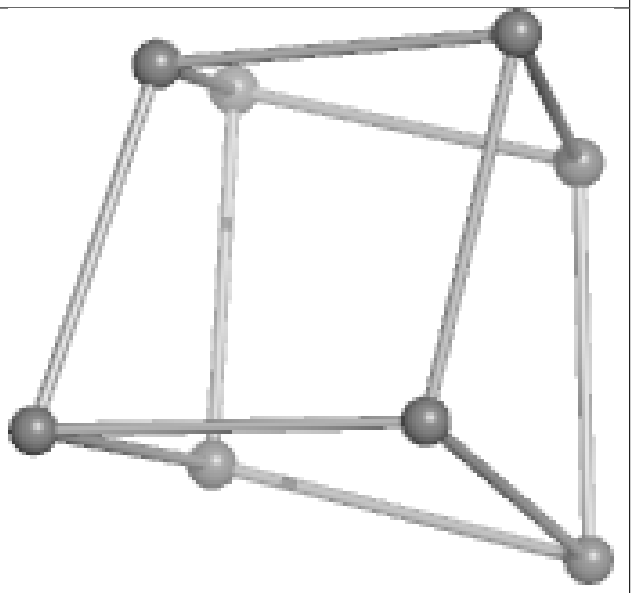

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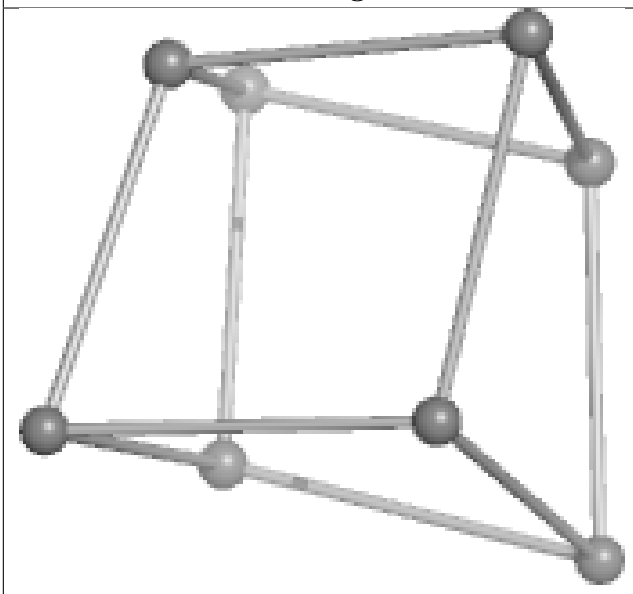

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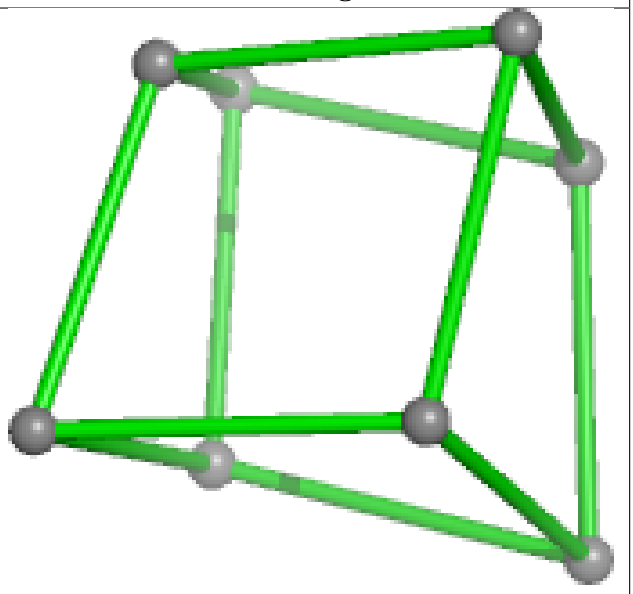
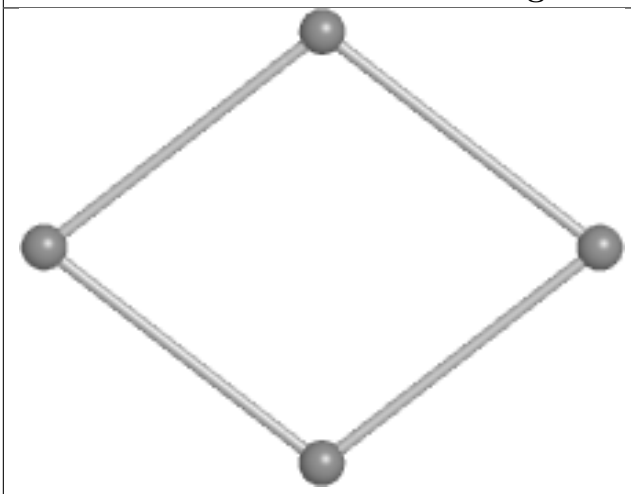


Rings

Ligand FES K 602



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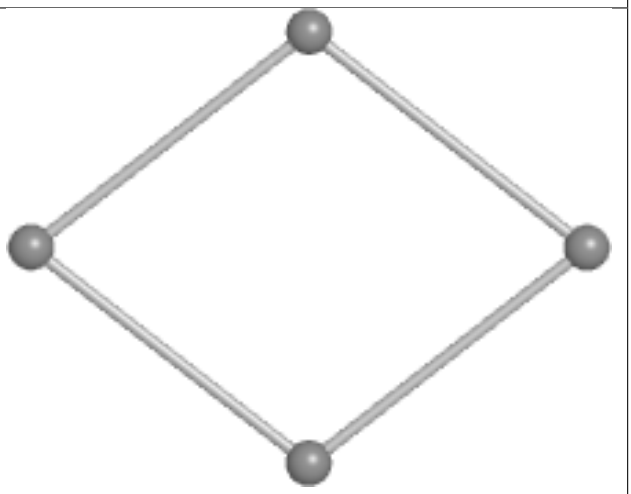
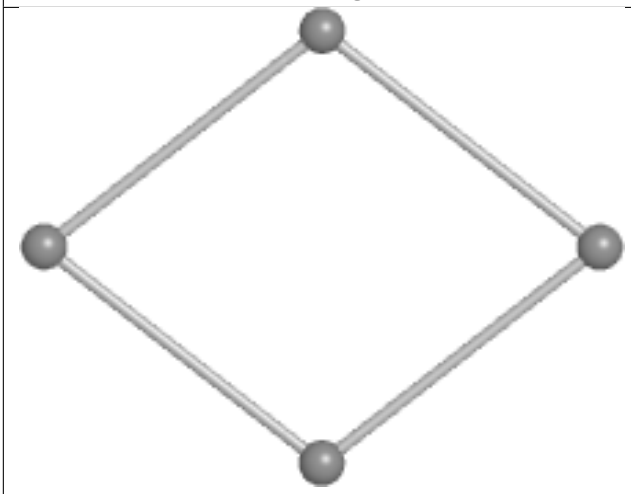


Bond angles



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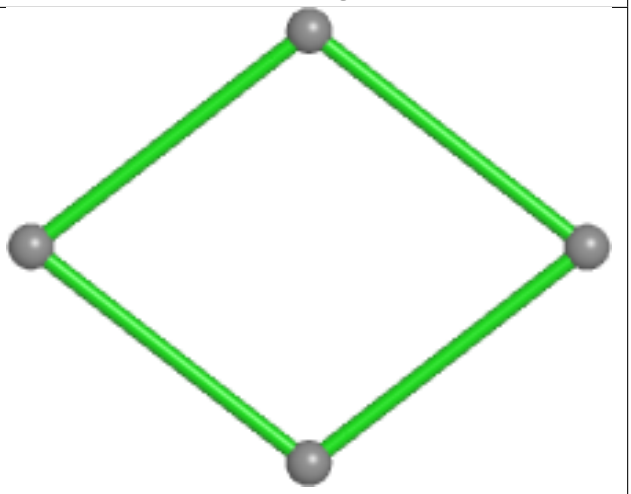
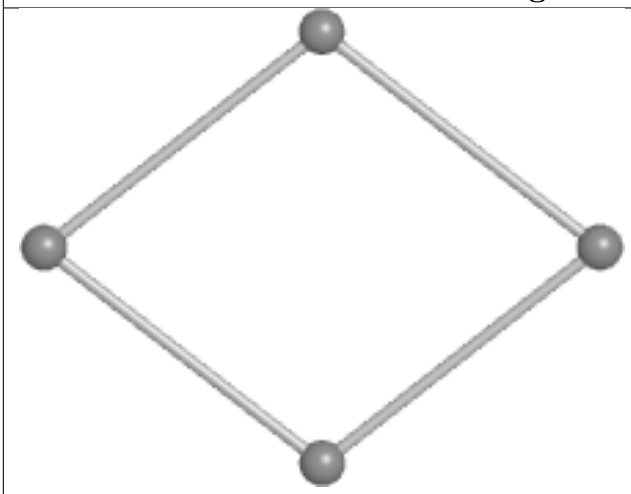


Rings

Ligand FES B 602



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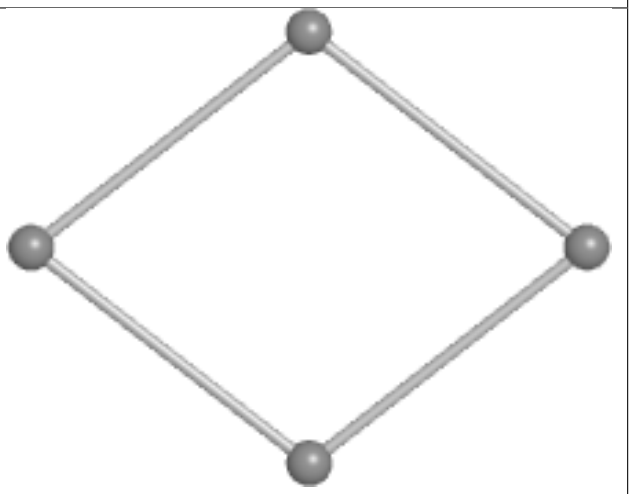

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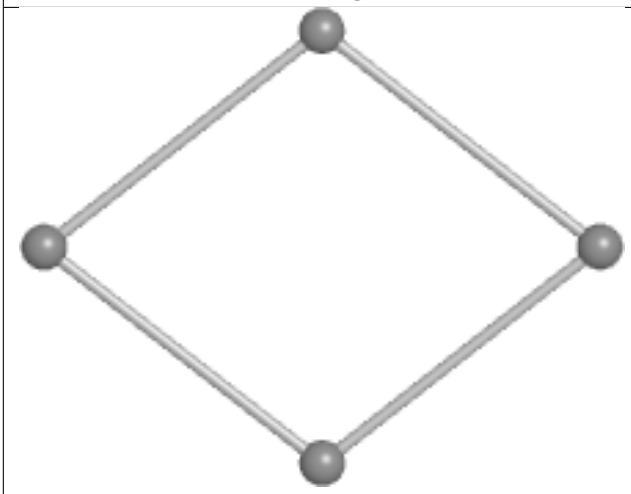

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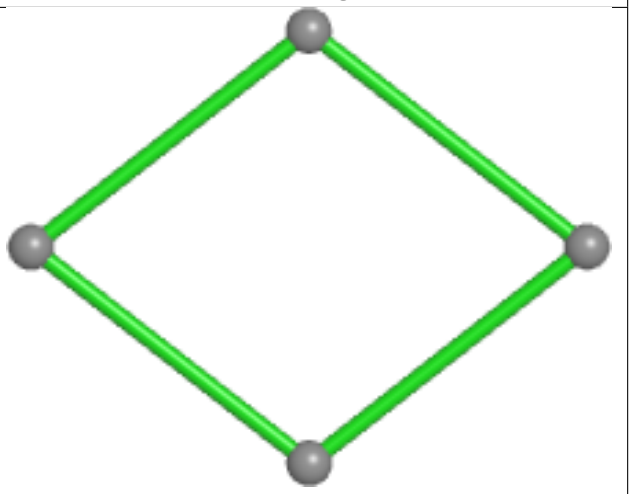
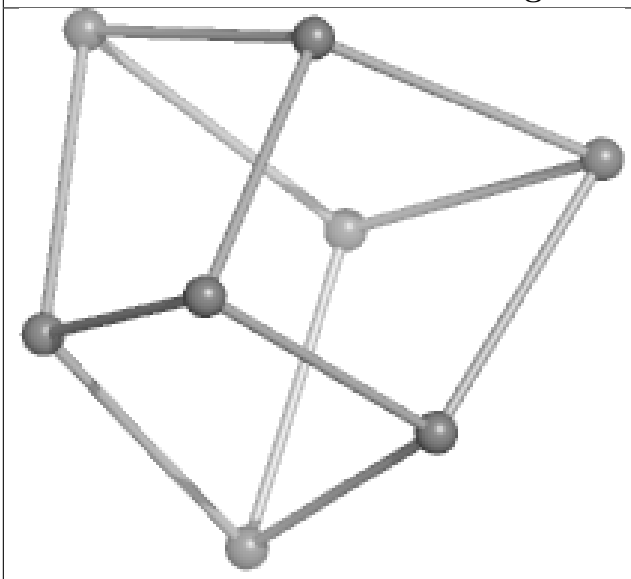


Rings

Ligand SF4 L 1206



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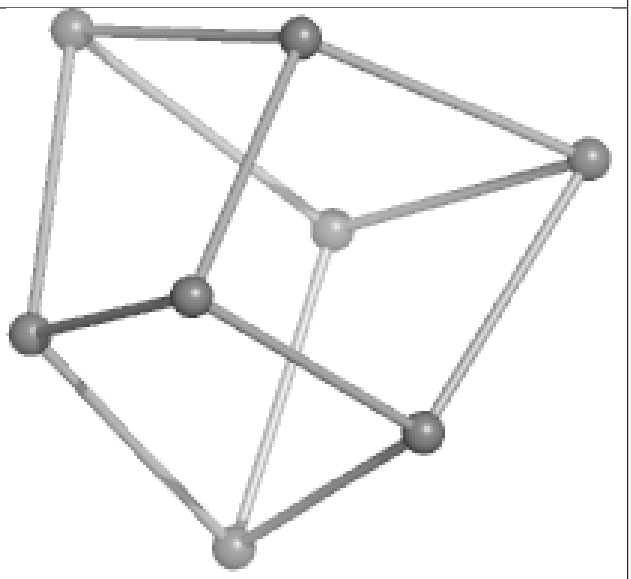

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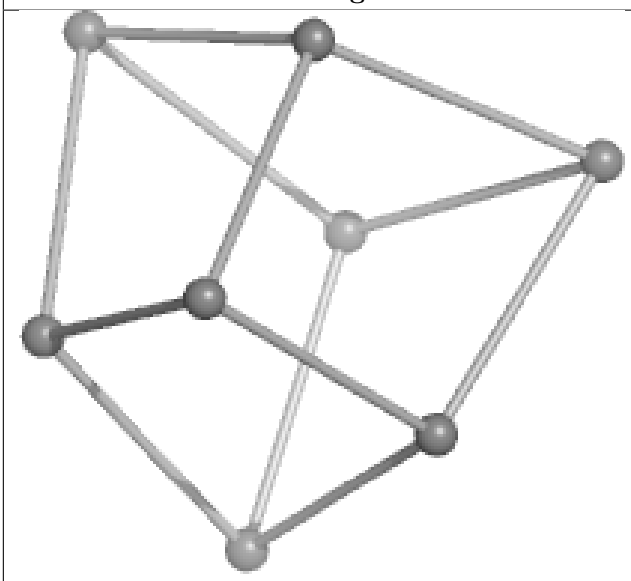

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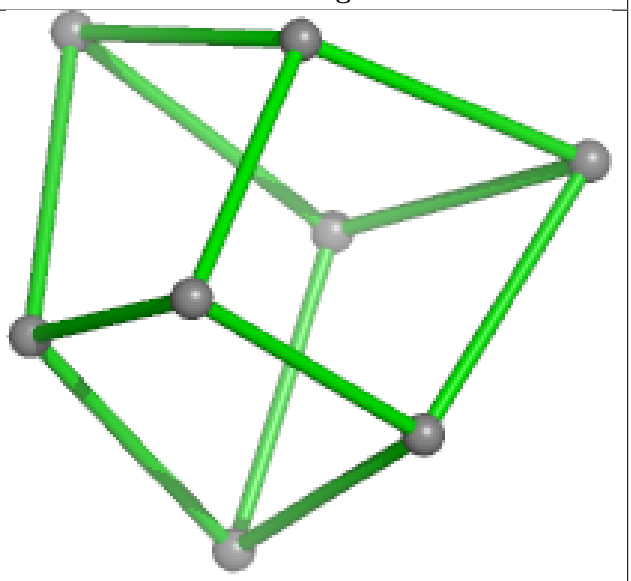
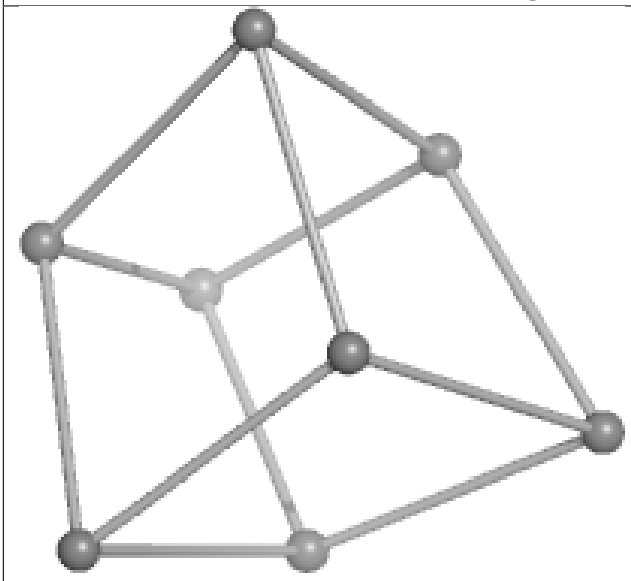


Rings

Ligand SF4 F 1206



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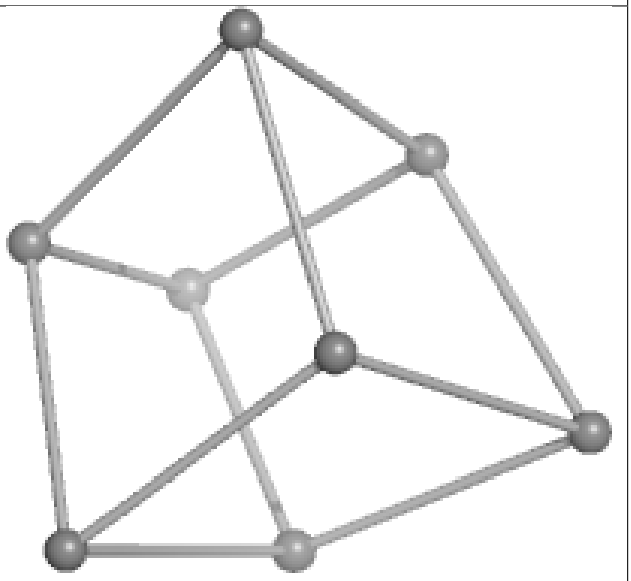
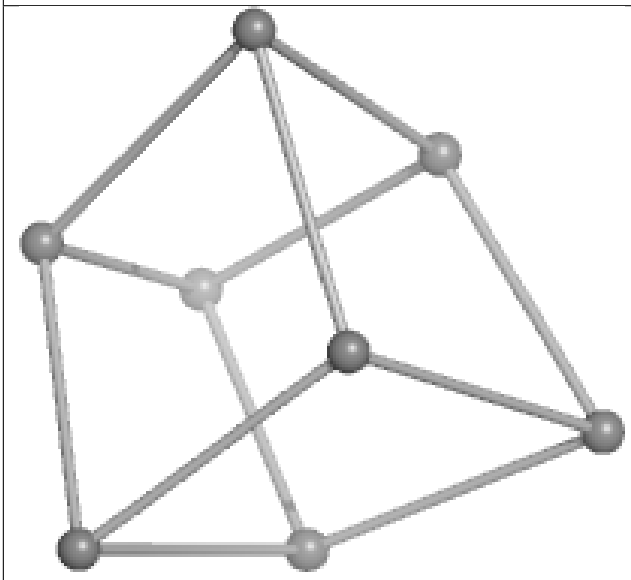


Bond angles



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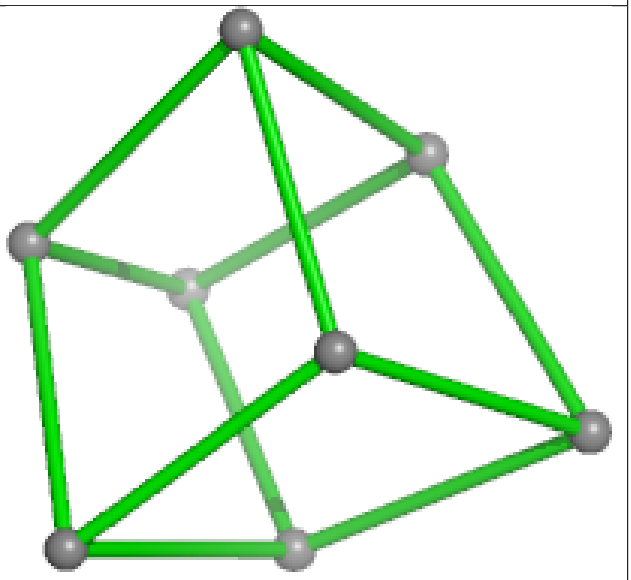
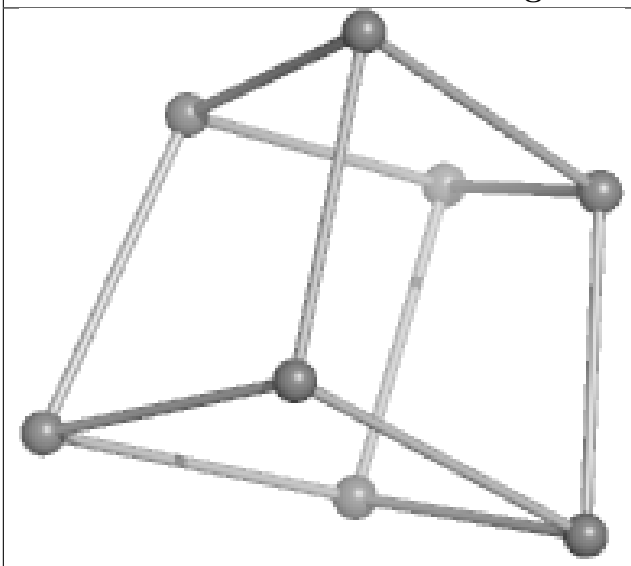


Rings

Ligand SF4 L 1208



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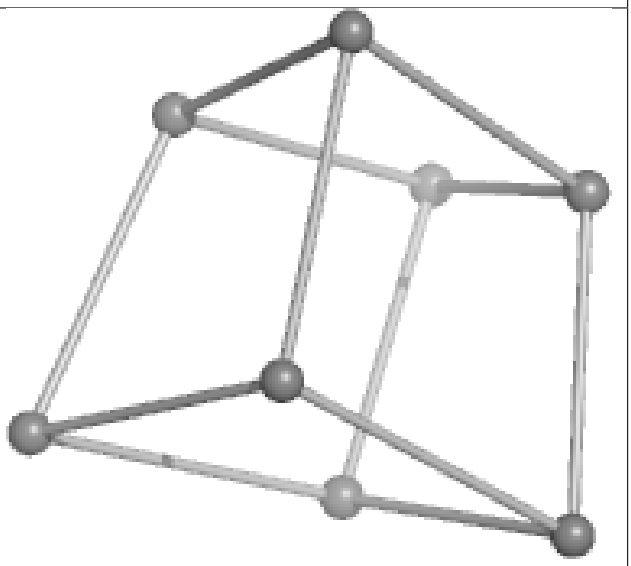
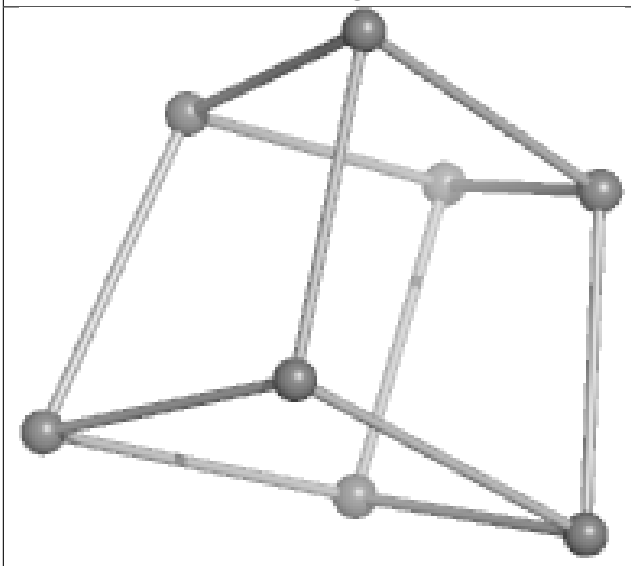


Bond angles



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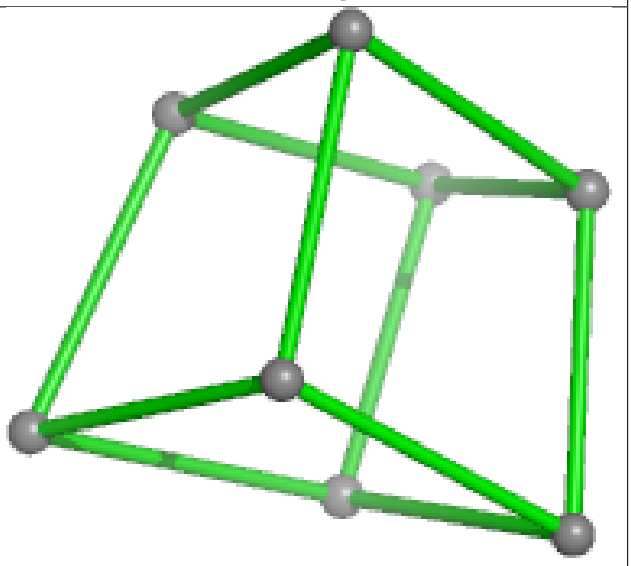
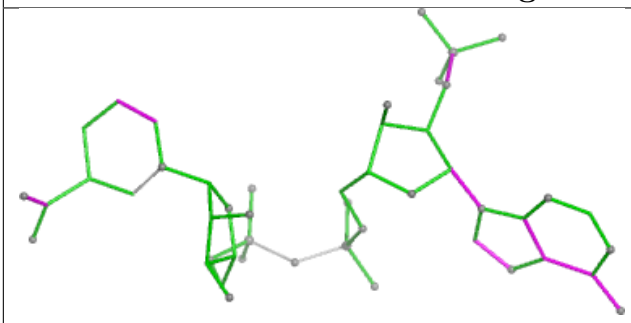


Rings

Ligand NDP I 1203



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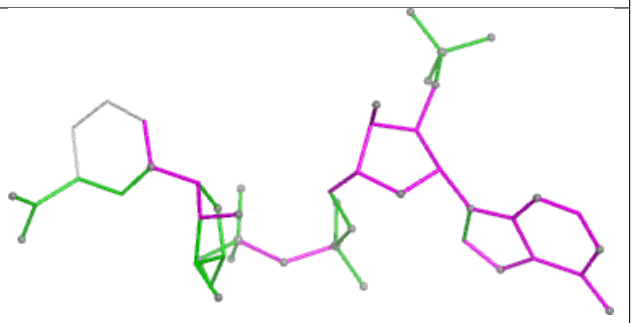
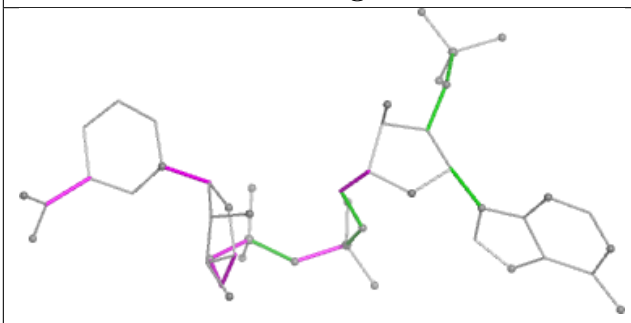


Bond angles



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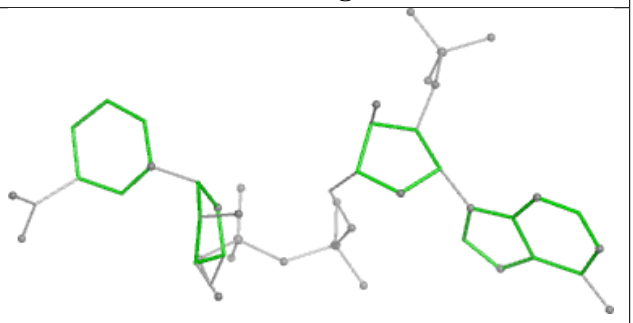
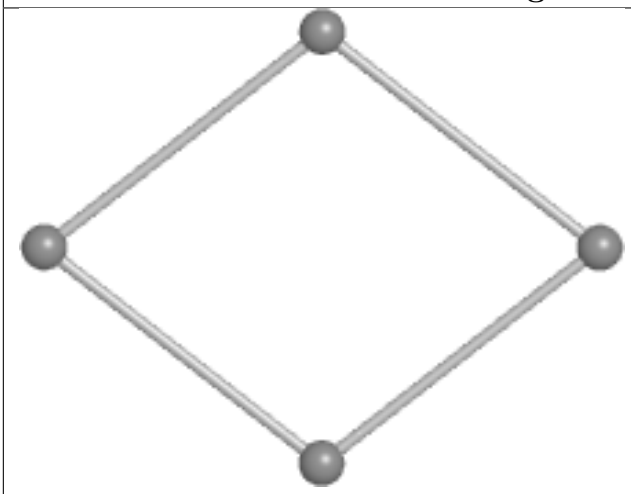


Rings

Ligand FES H 602



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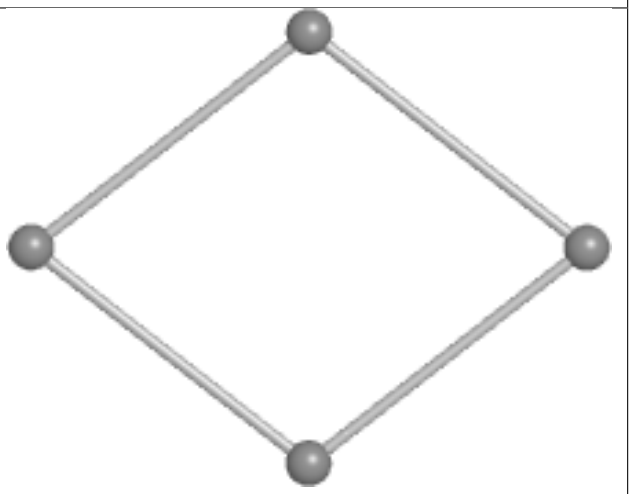
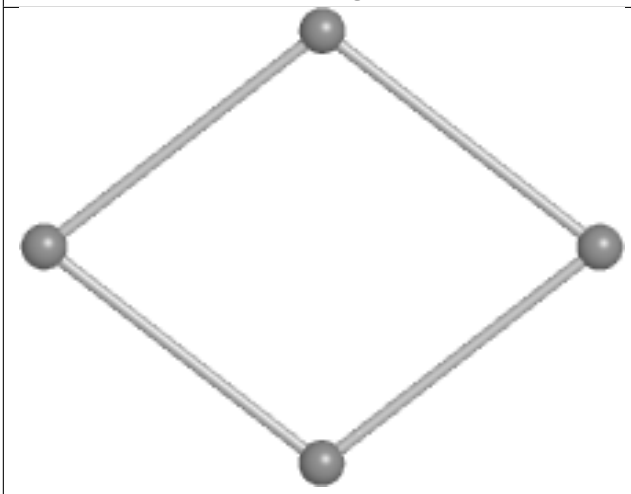


Bond angles



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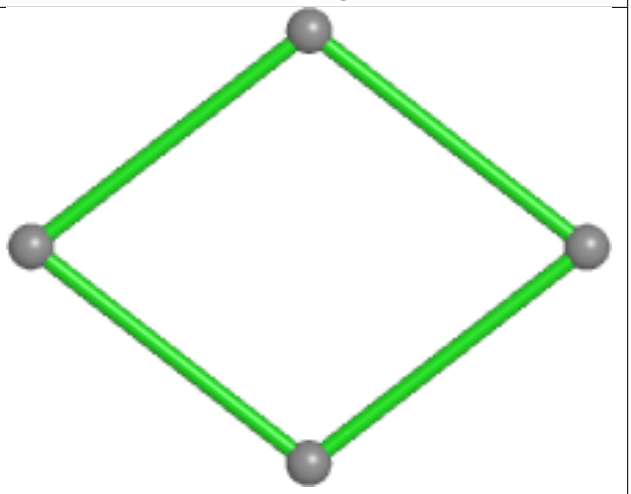
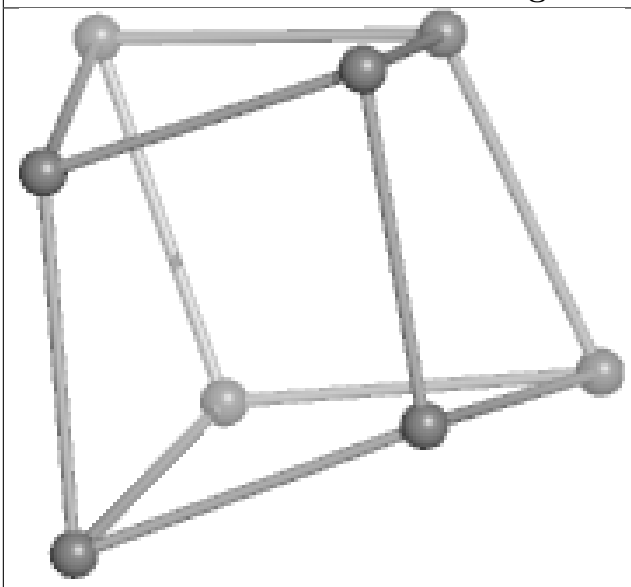
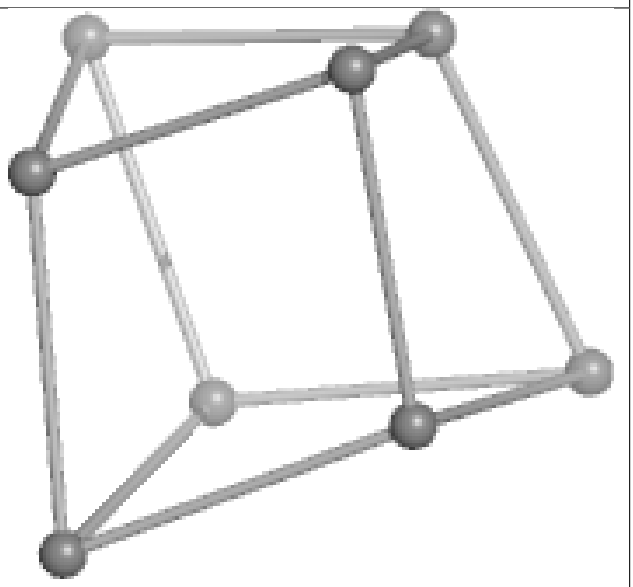


Rings

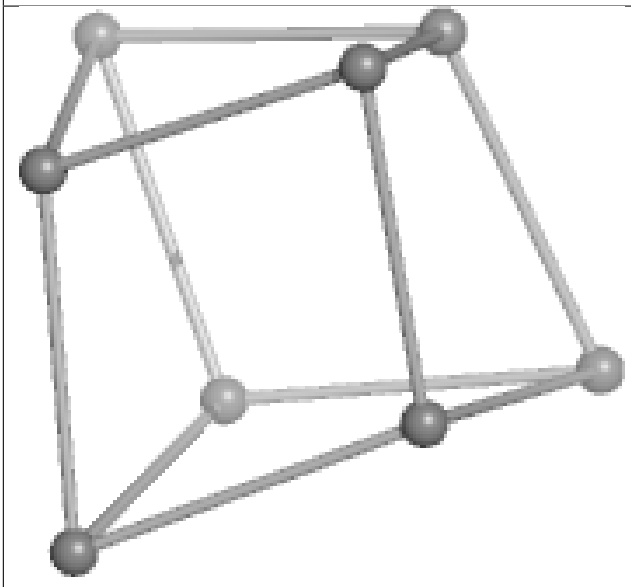
Ligand SF4 I 1202



Bond lengths



Bond angles



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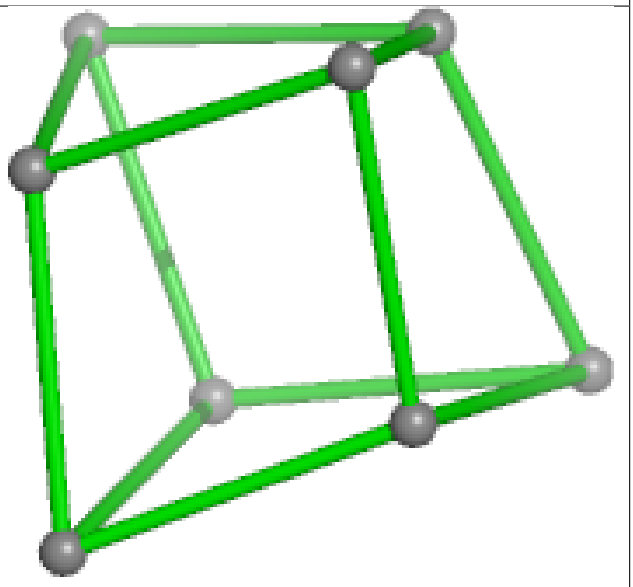
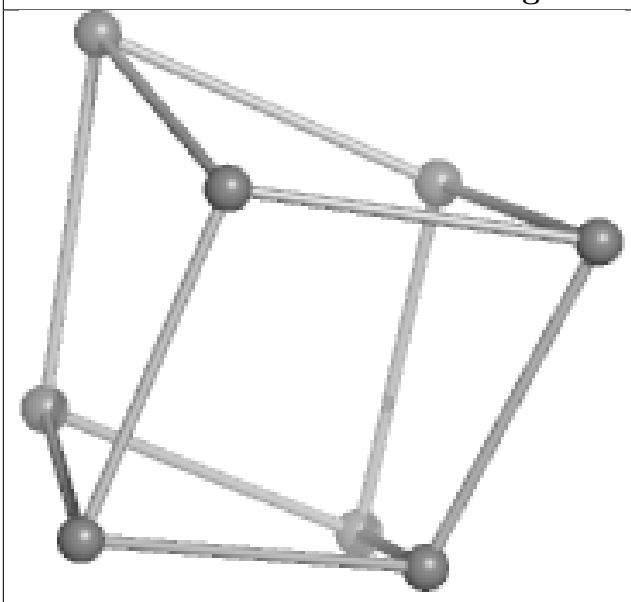
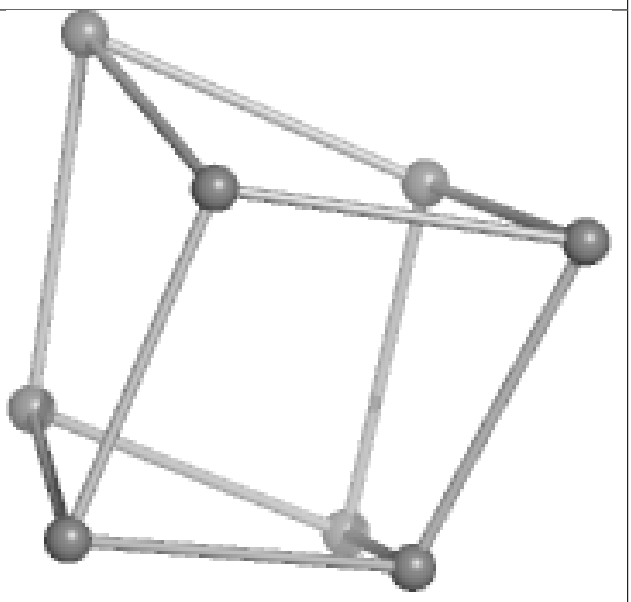


Rings

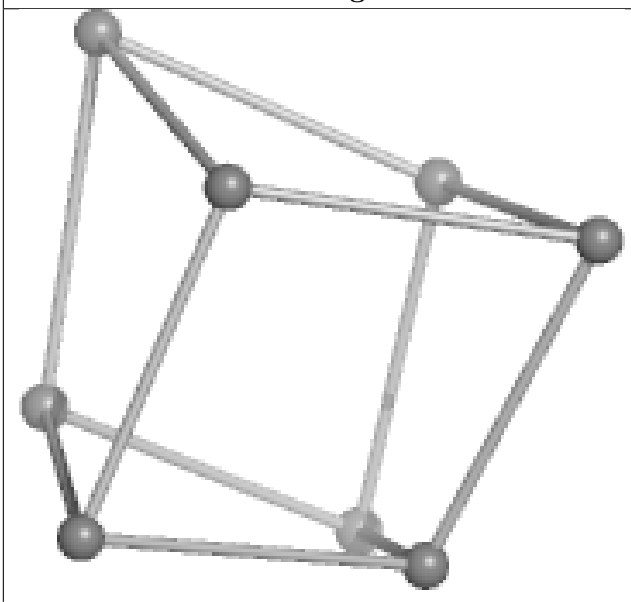
Ligand SF4 C 1202



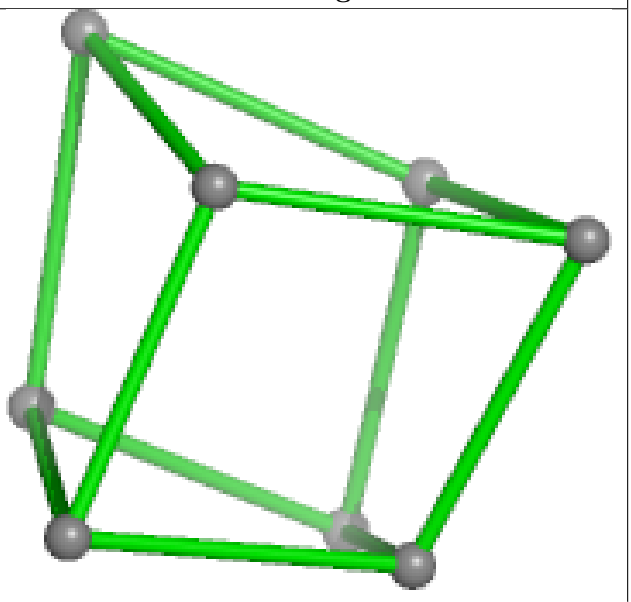
Bond lengths



Bond angles

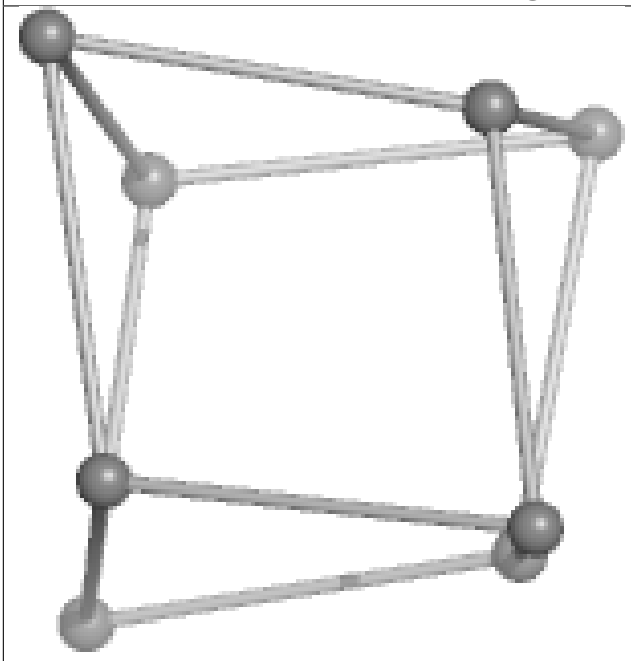


Torsions



Rings

Ligand SF4 F 1207



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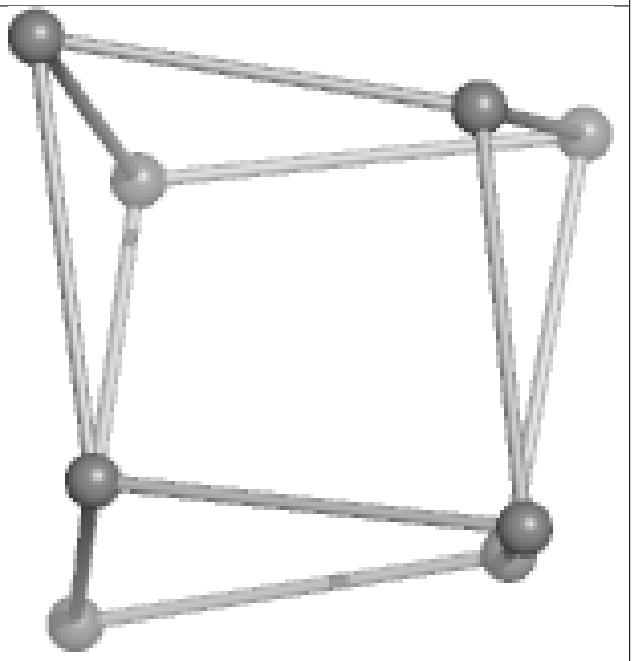
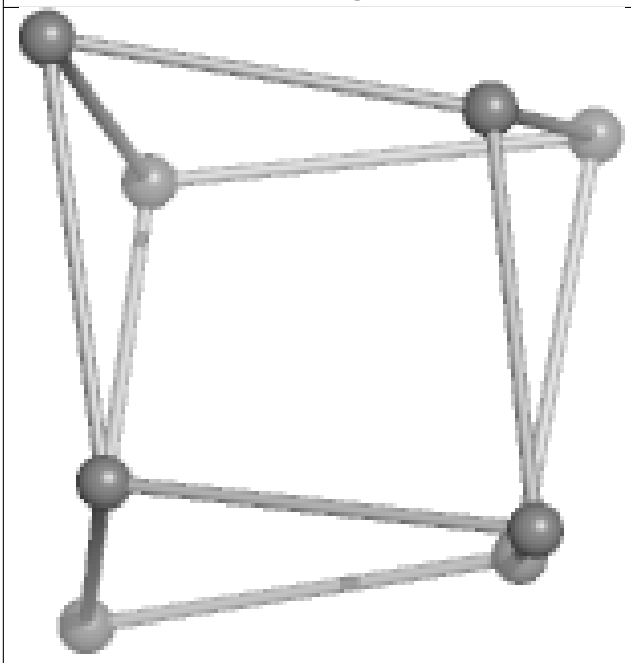


Bond angles



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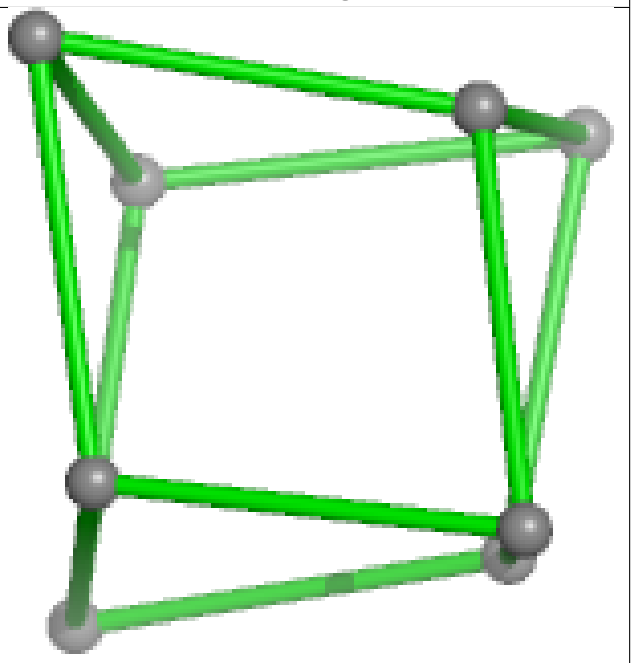
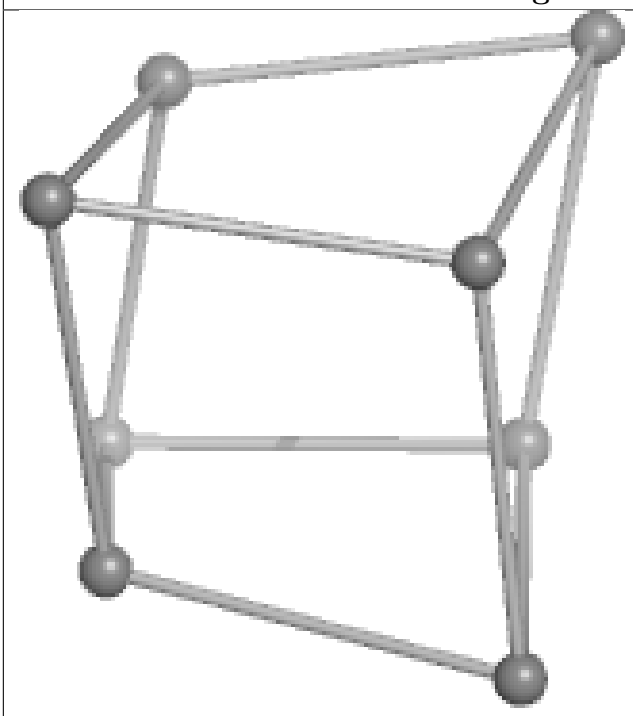


Rings

Ligand SF4 E 607



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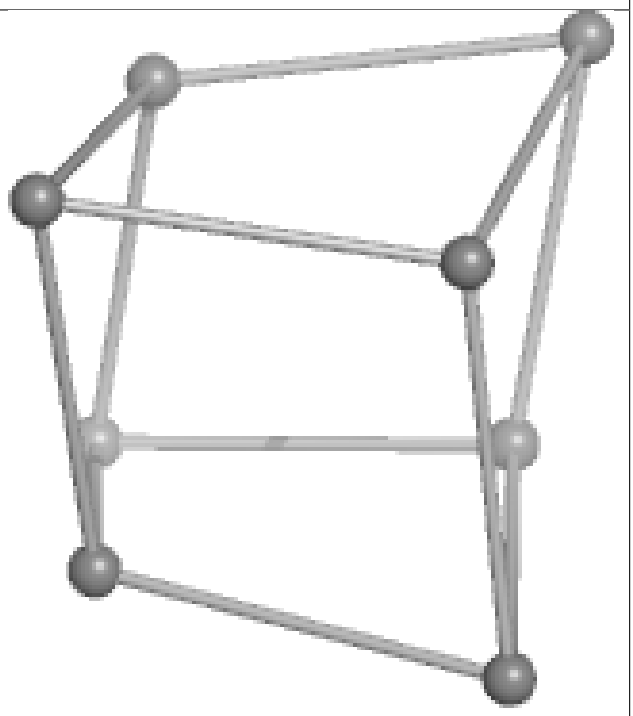
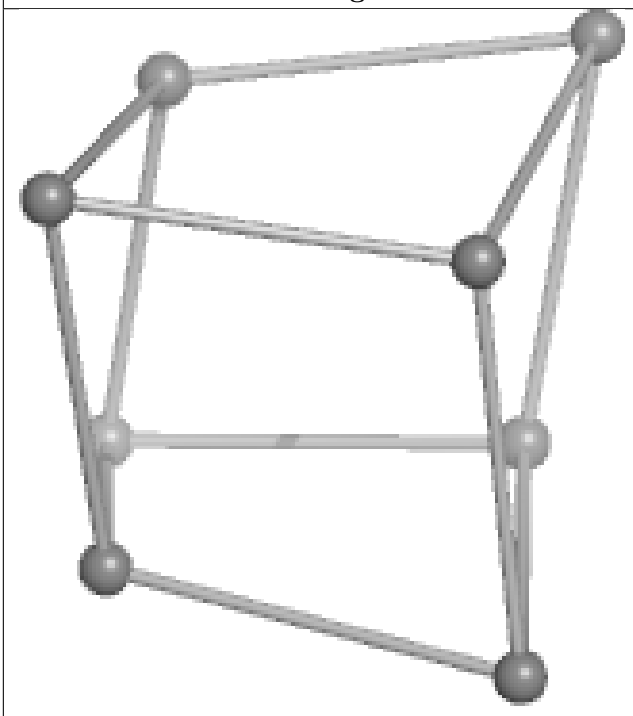


Bond angles



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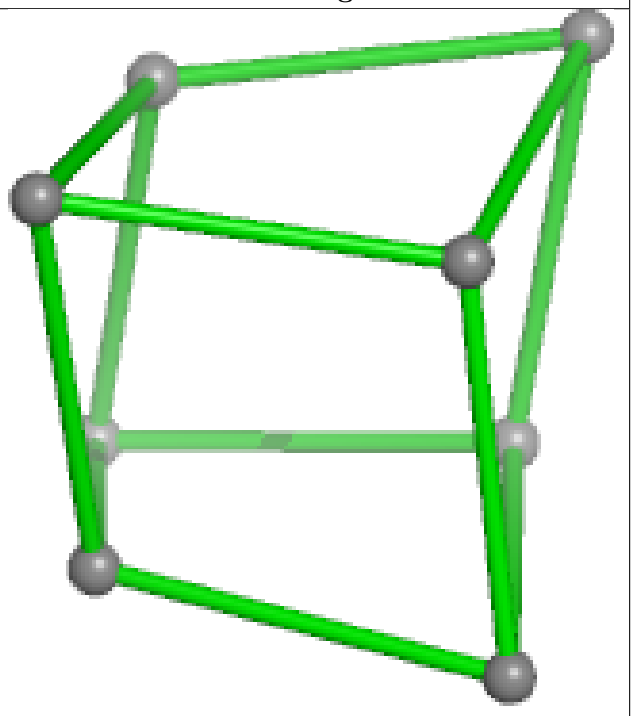
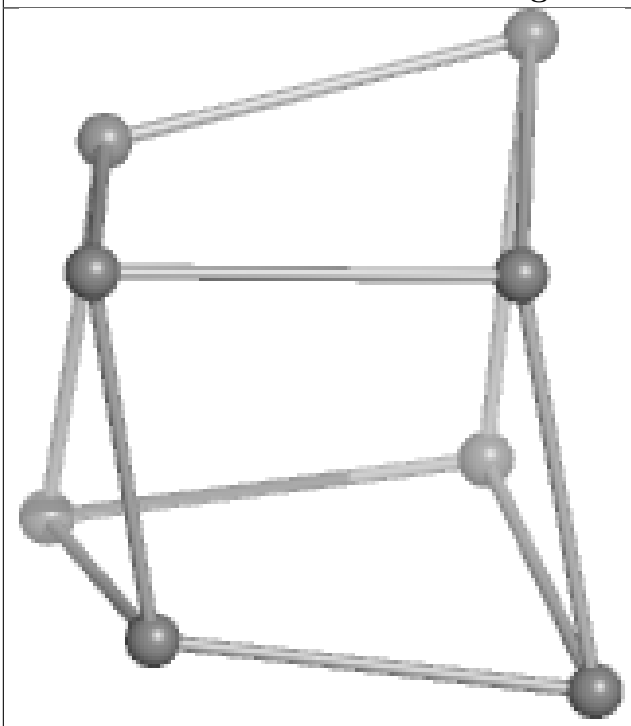


Rings

Ligand SF4 K 607



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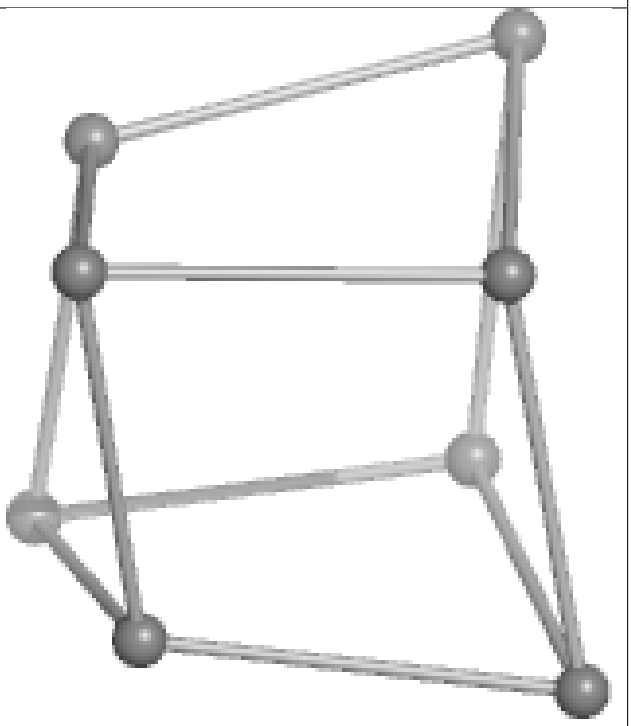
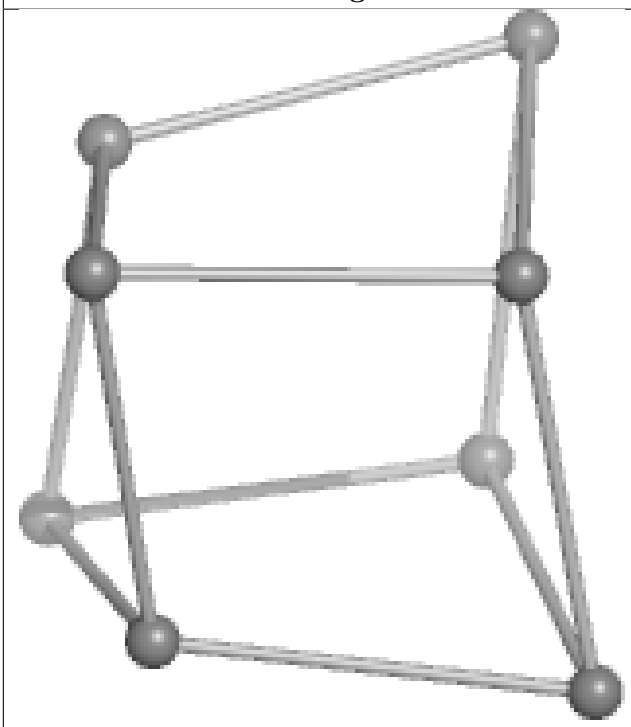


Bond angles



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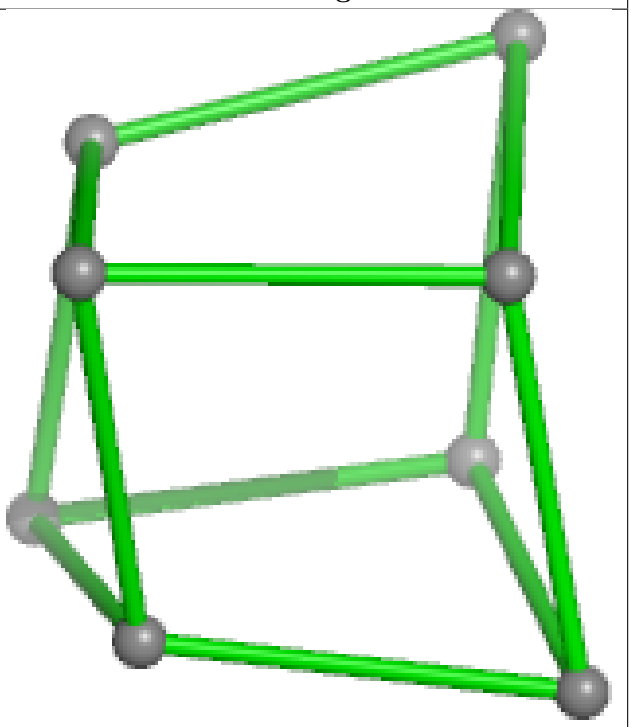
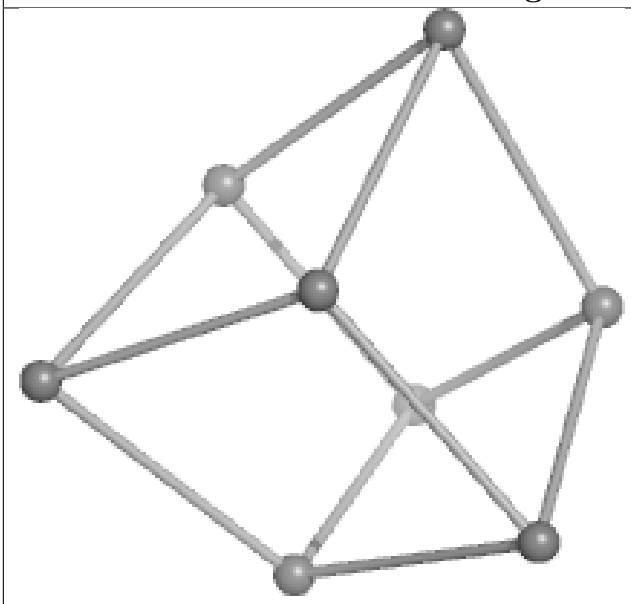


Rings

Ligand SF4 L 1205



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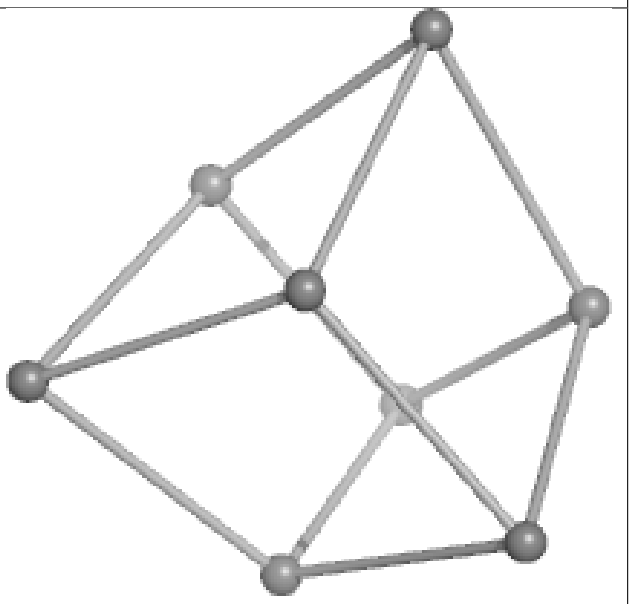
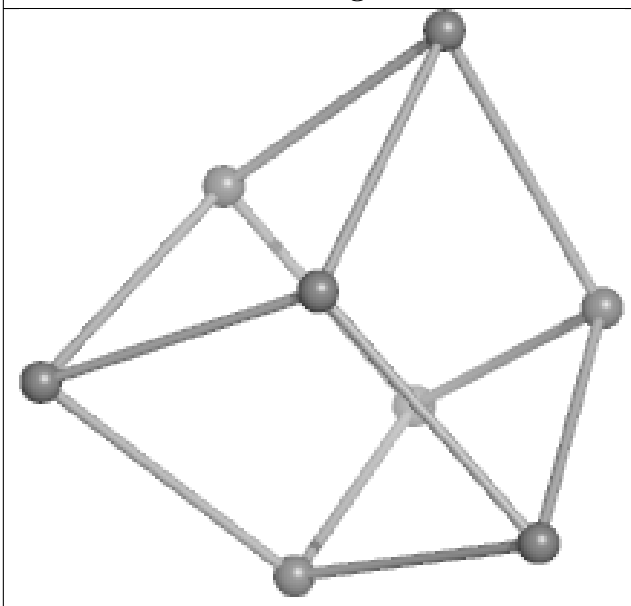


Bond angles



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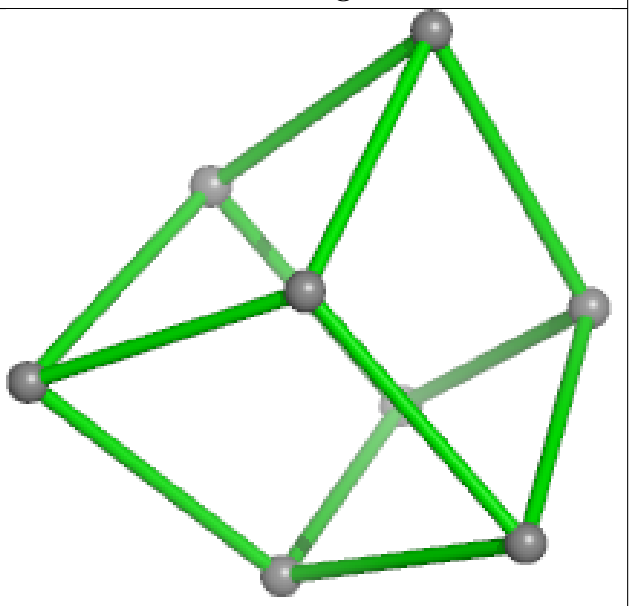
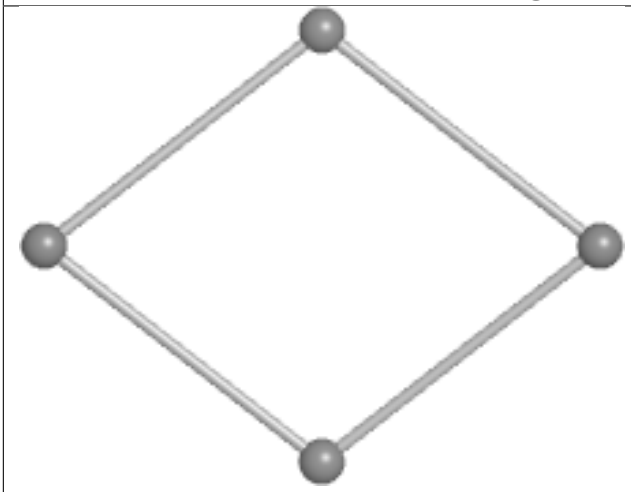


Rings

Ligand FES G 201



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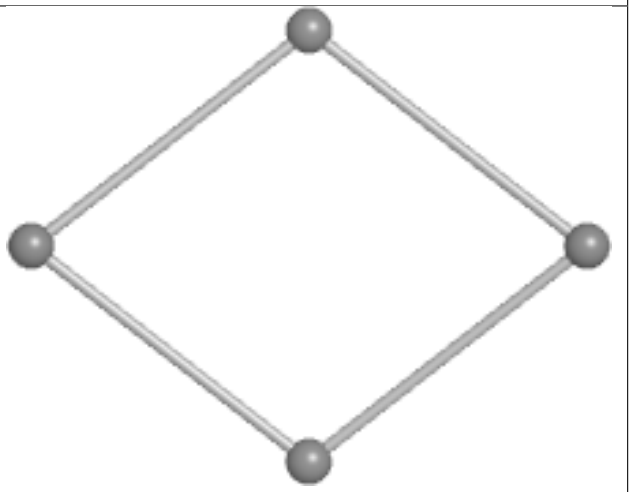
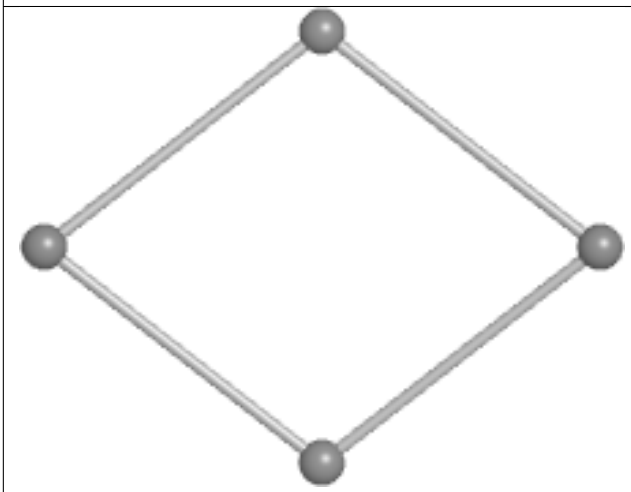


Bond angles



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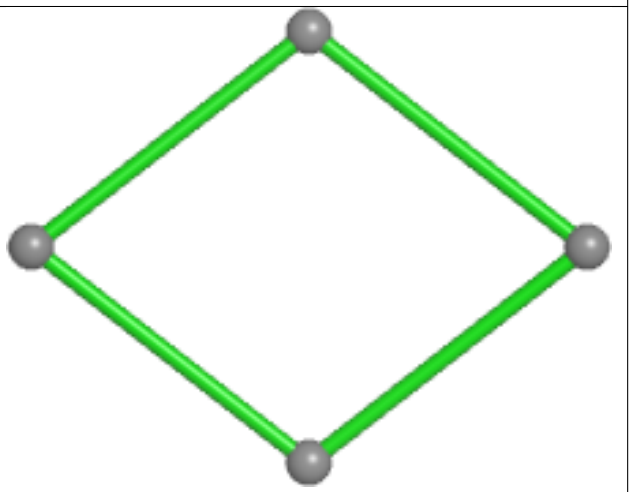
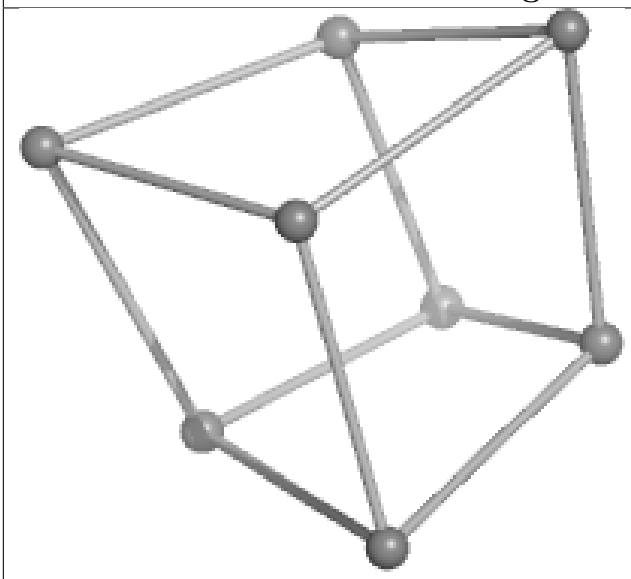


Rings

Ligand SF4 C 1206



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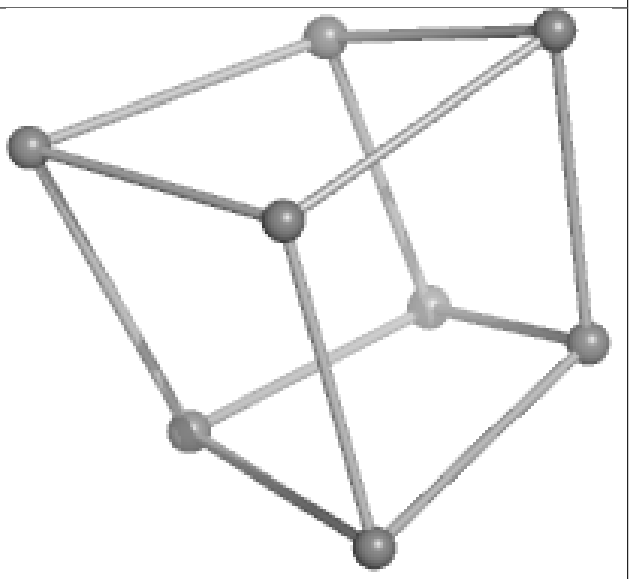
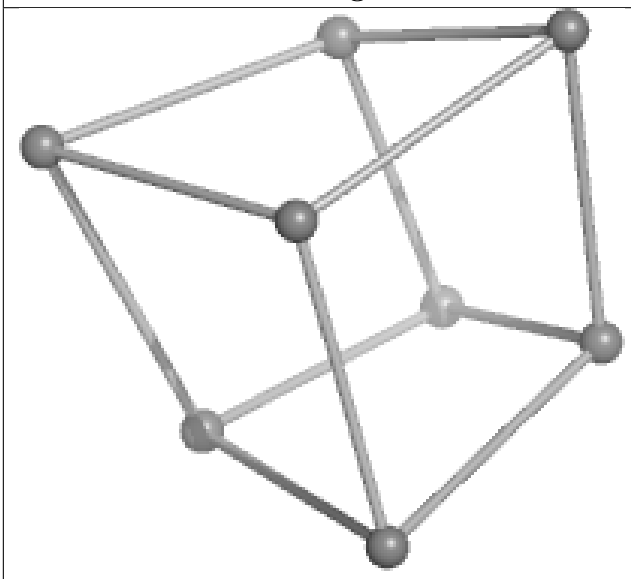


Bond angles



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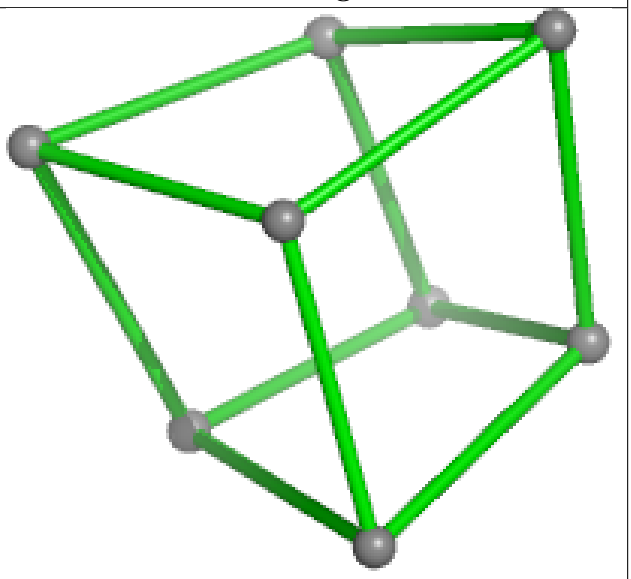
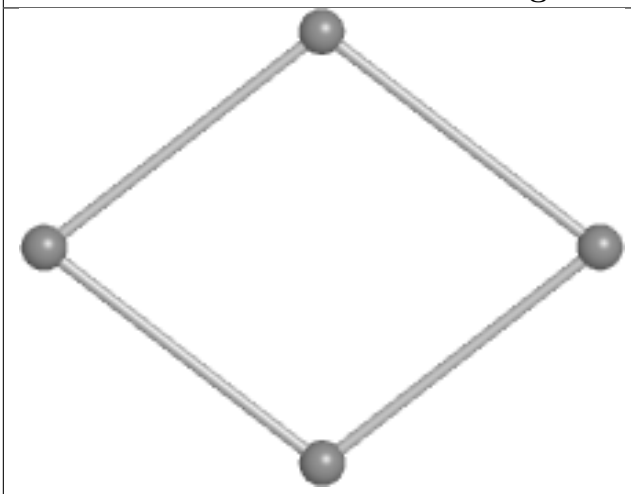


Rings

Ligand FES E 602



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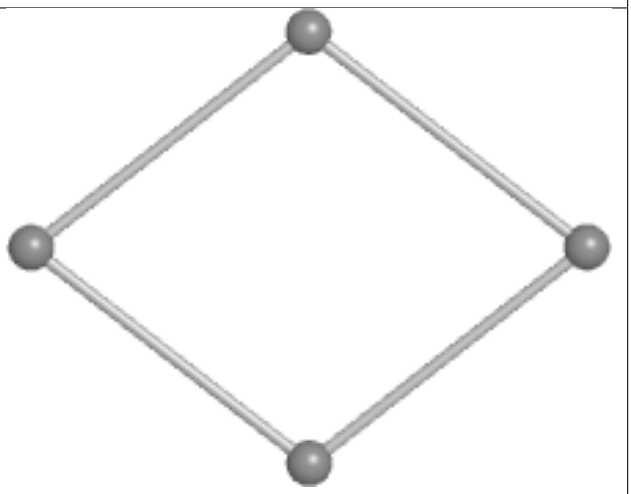

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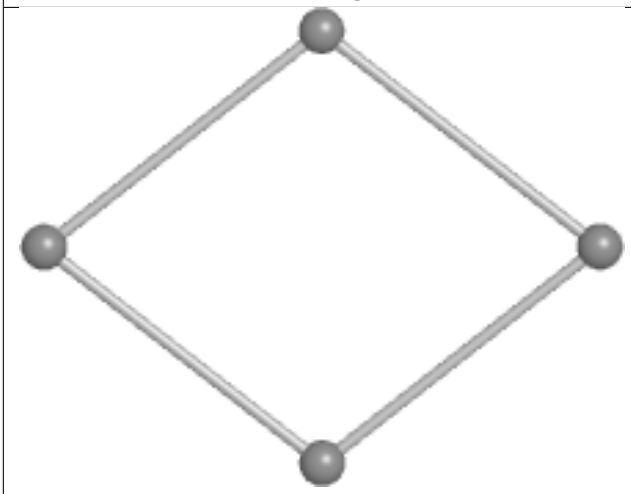

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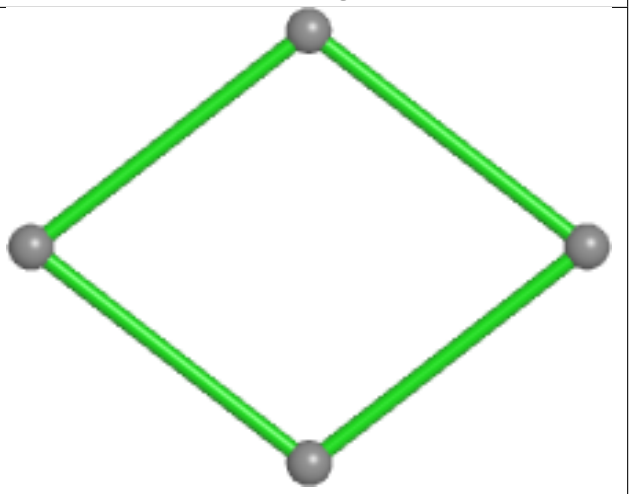
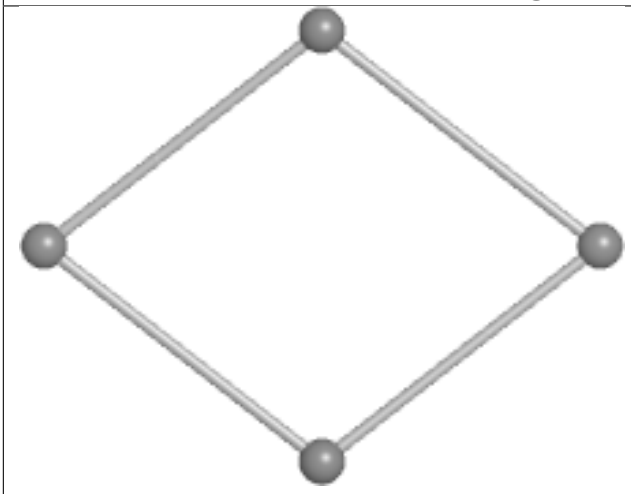


Rings

Ligand FES D 201



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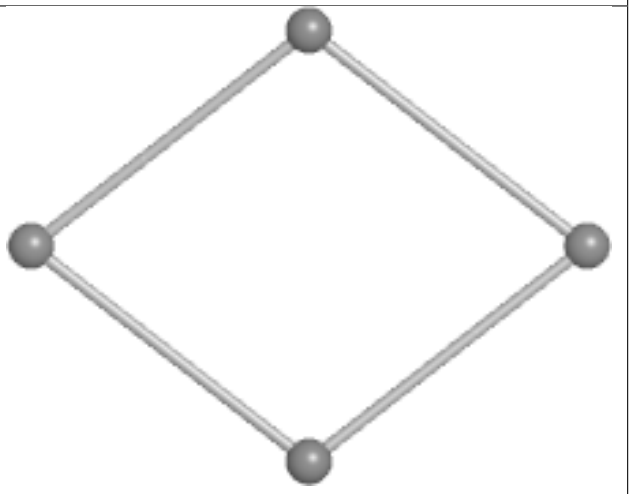
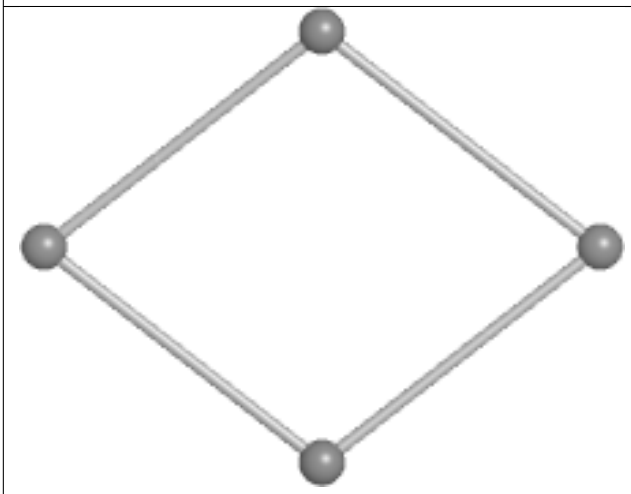


Bond angles



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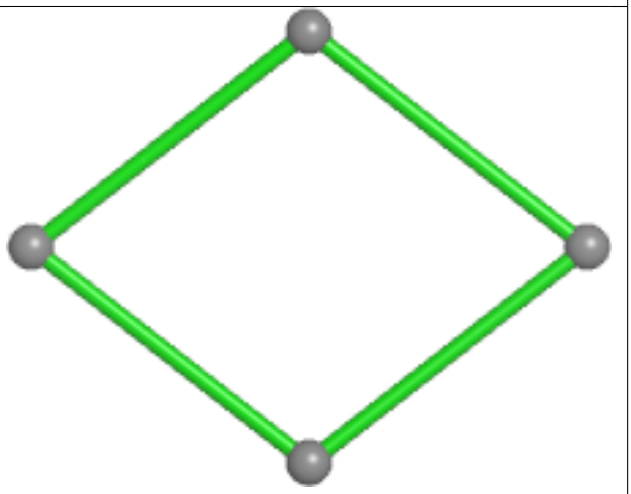
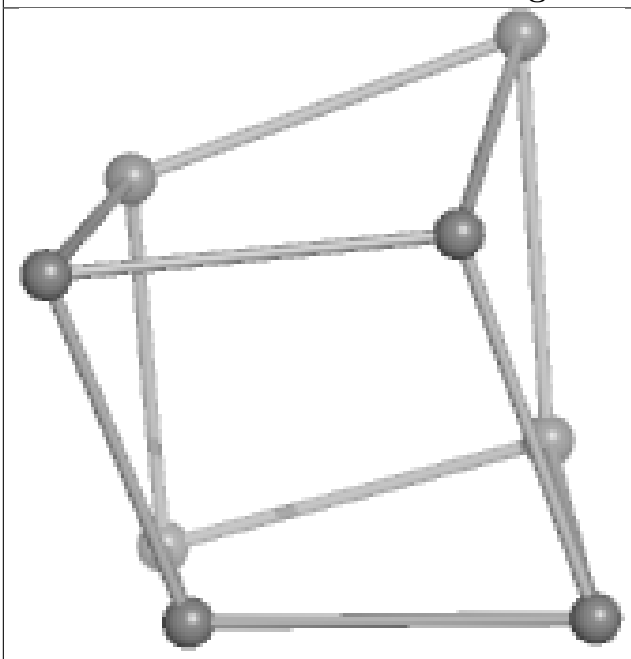


Rings

Ligand SF4 I 1207



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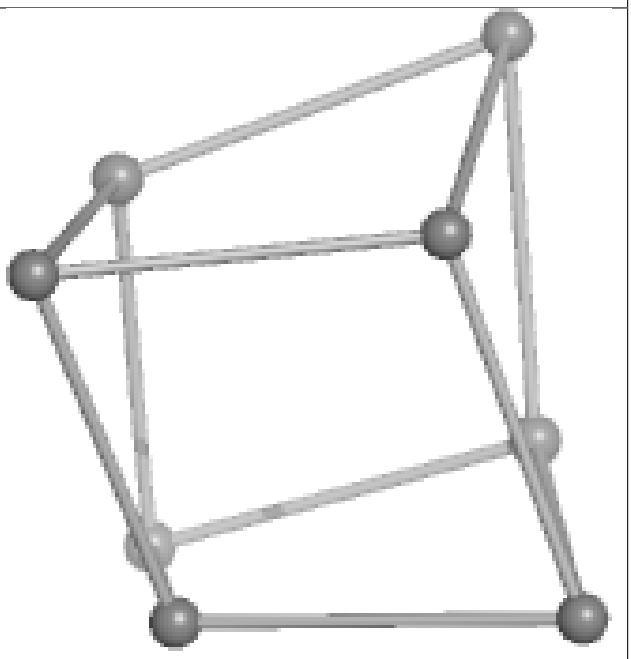

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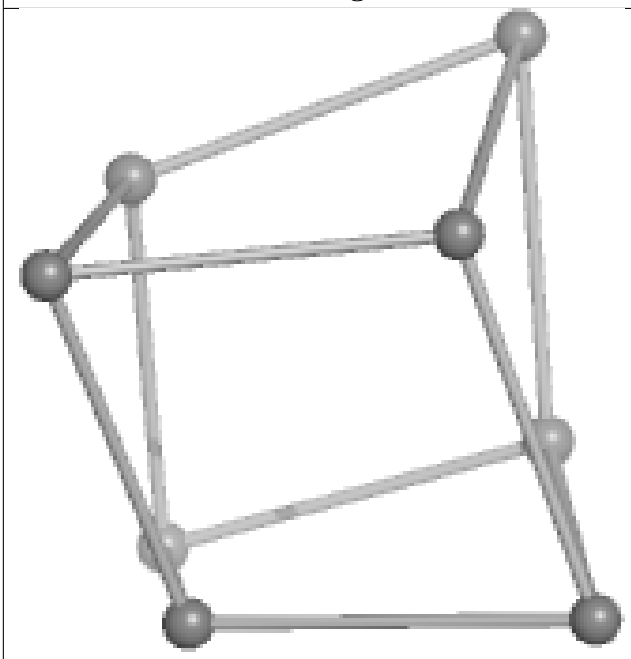

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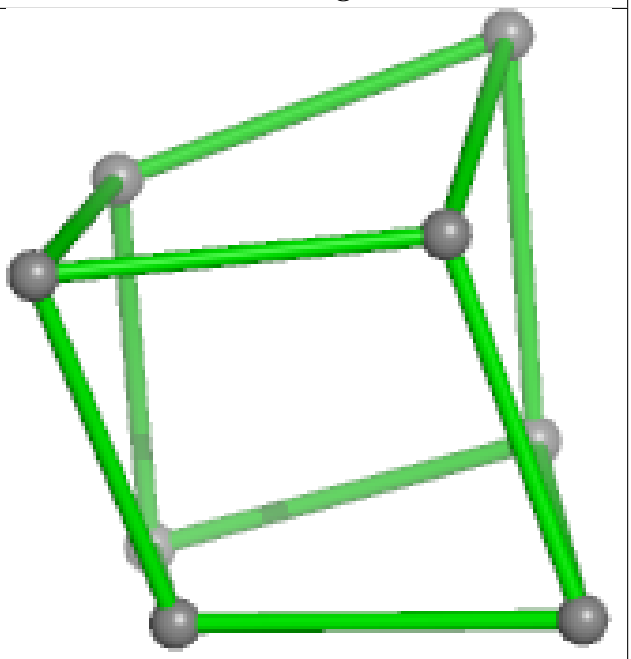
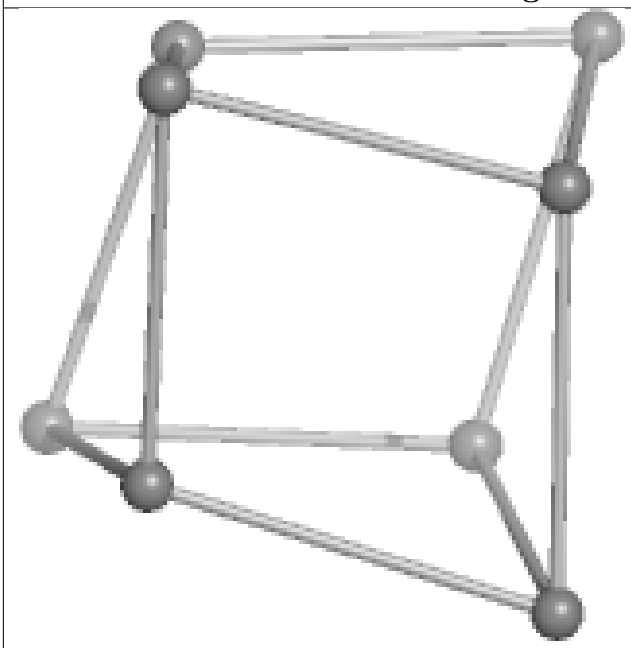


Rings

Ligand SF4 C 1207



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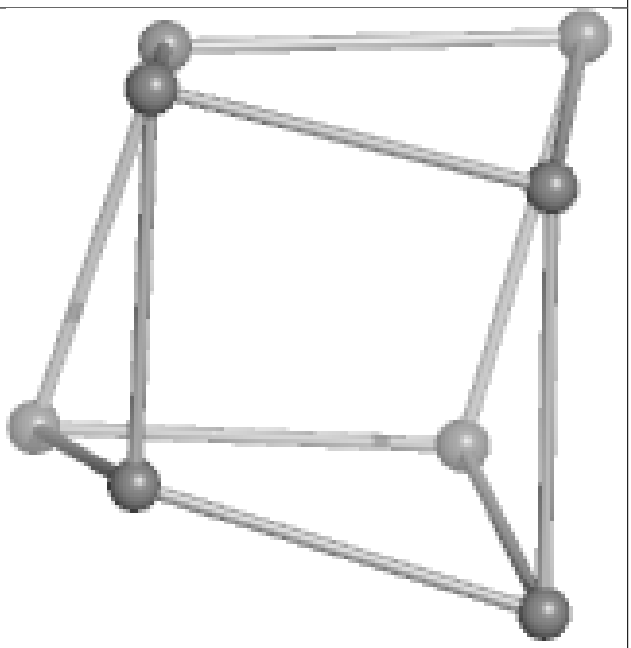
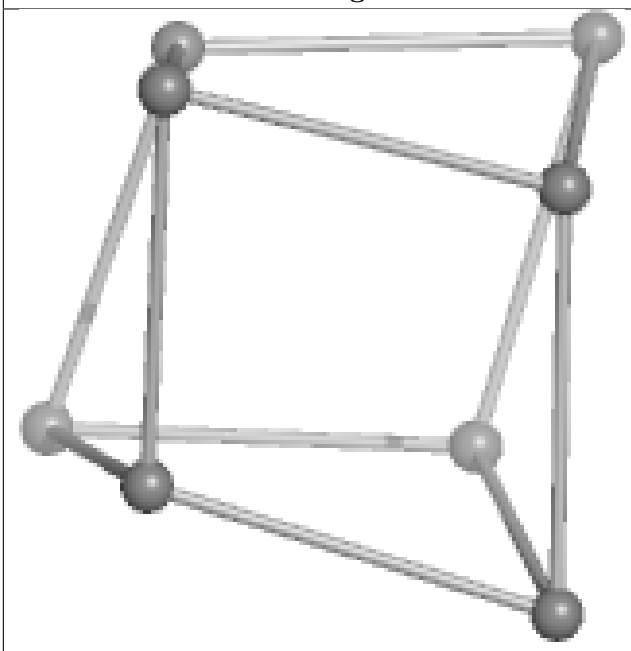


Bond angles



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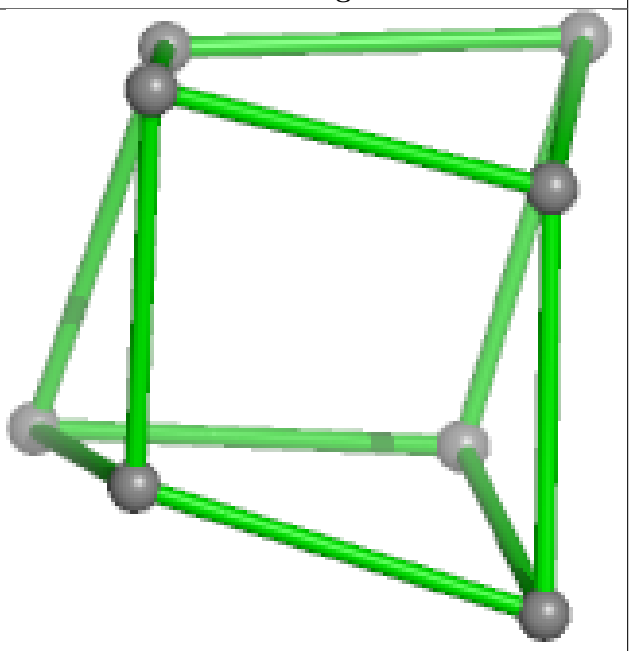
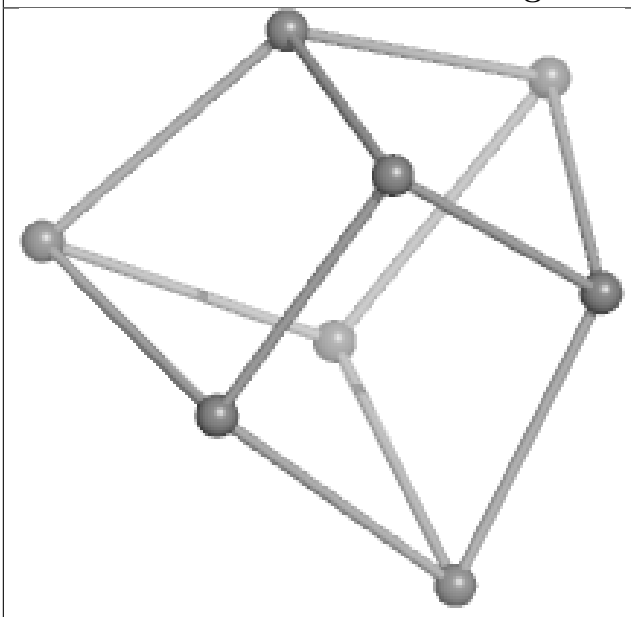


Rings

Ligand SF4 F 1205



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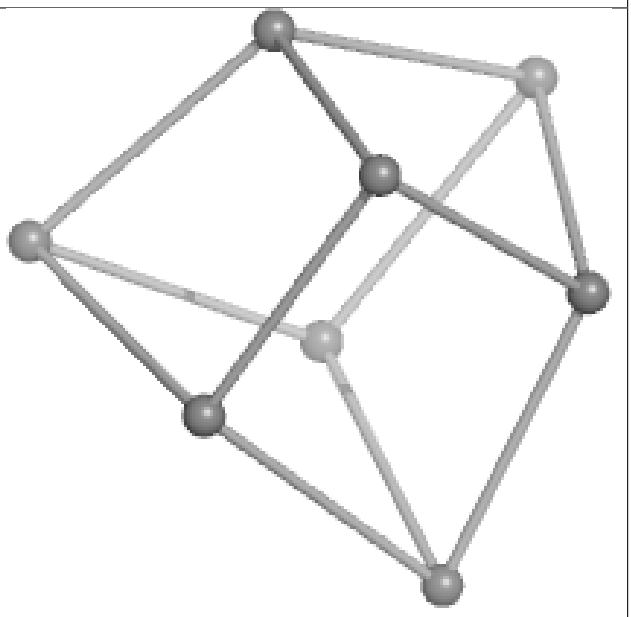
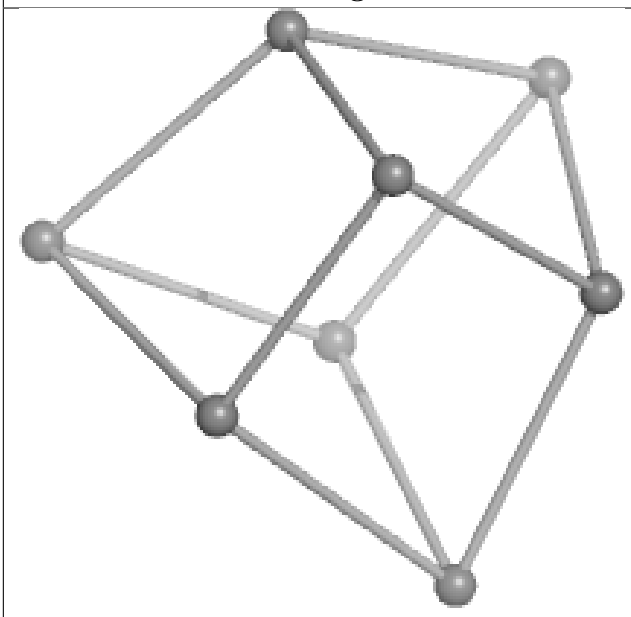


Bond angles



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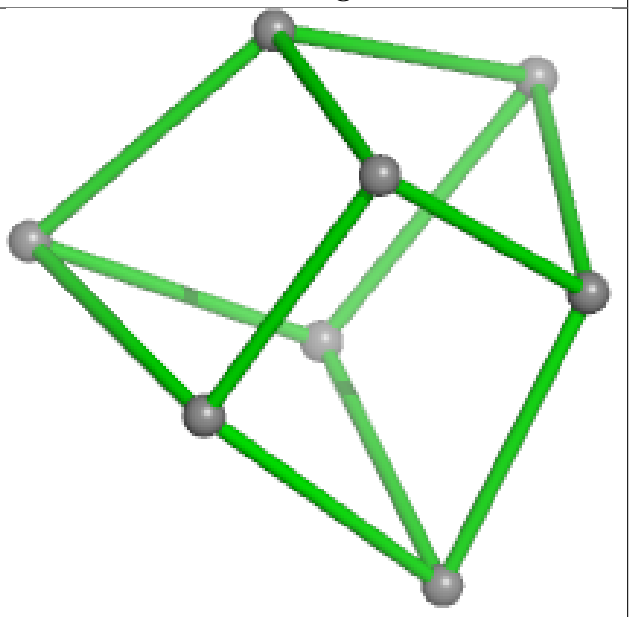
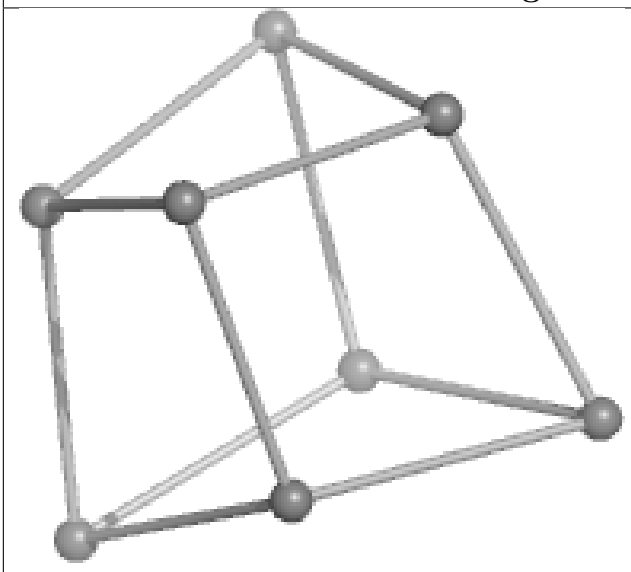


Rings

Ligand SF4 C 1208



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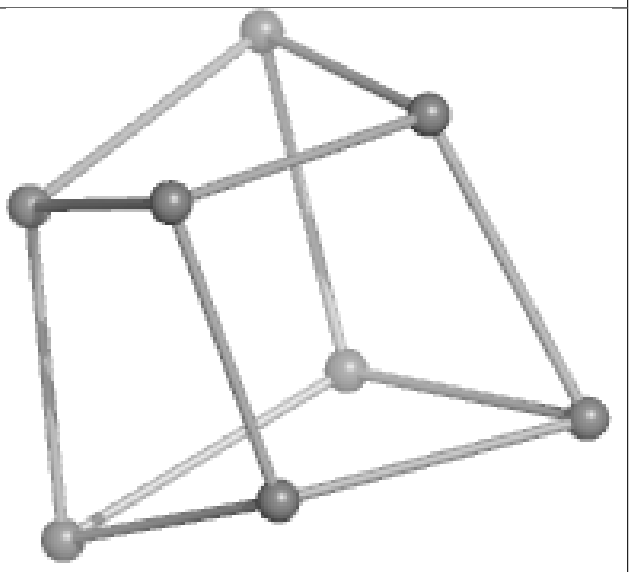
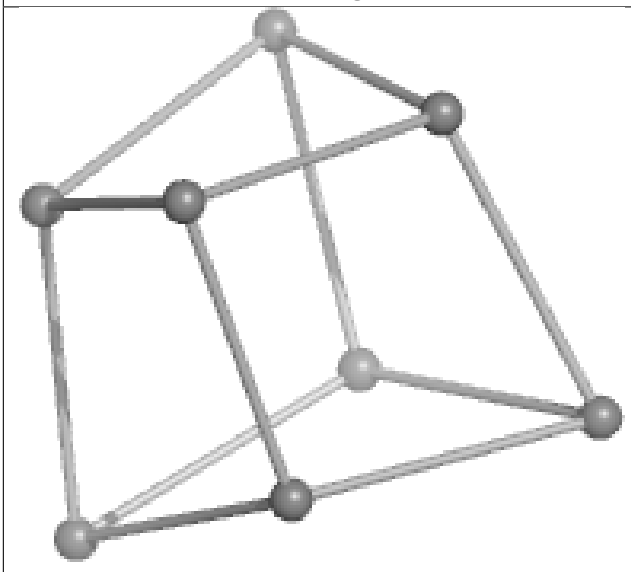


Bond angles



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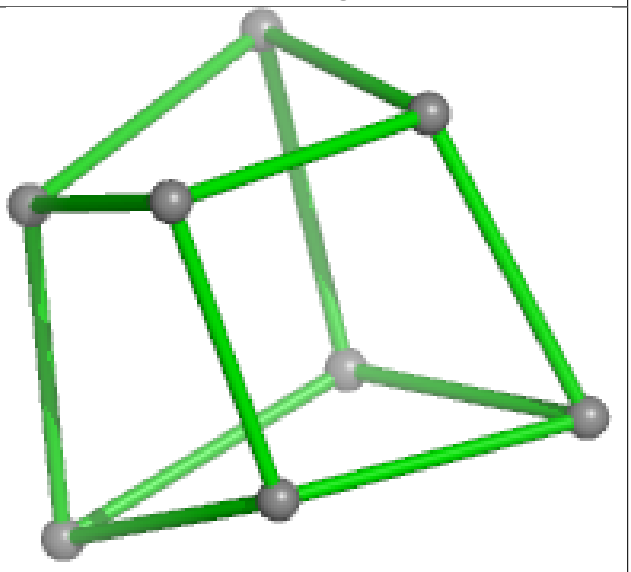


Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

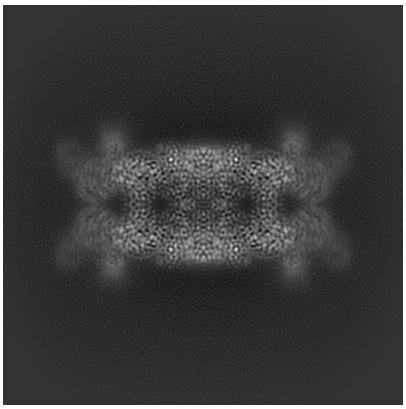
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16878. These allow visual inspection of the internal detail of the map and identification of artifacts.

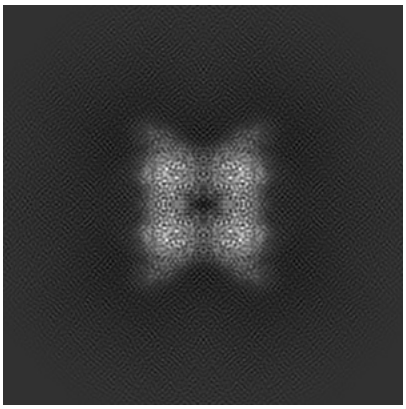
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

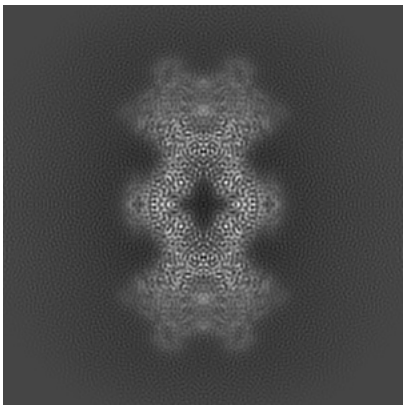
6.1.1 Primary map



X

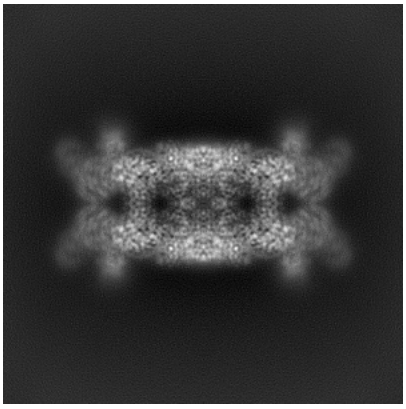


Y

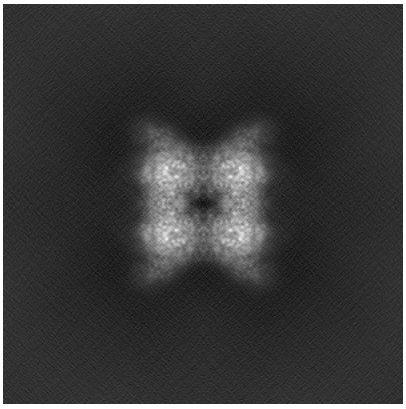


Z

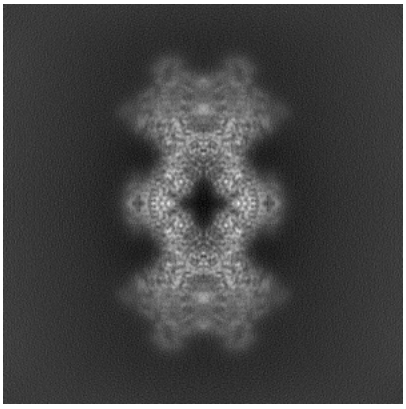
6.1.2 Raw map



X



Y

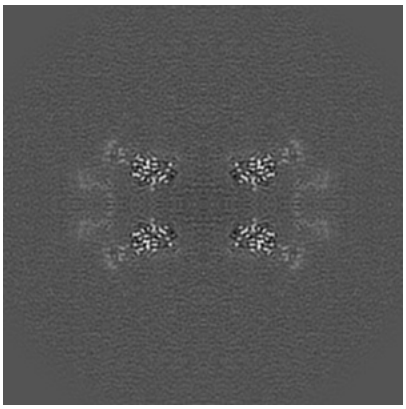


Z

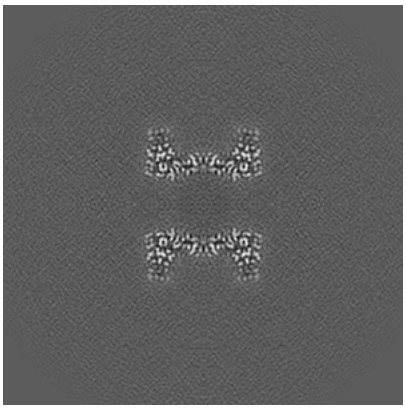
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

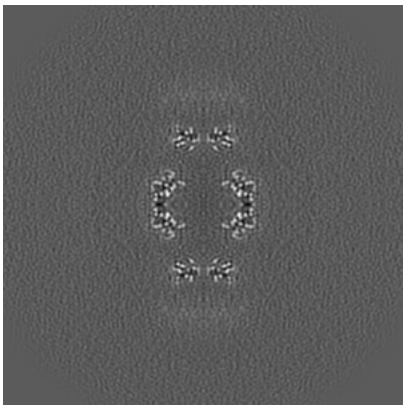
6.2.1 Primary map



X Index: 200

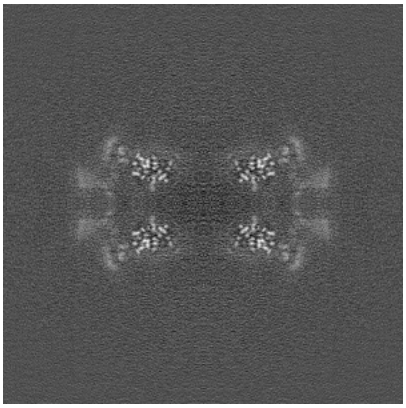


Y Index: 200

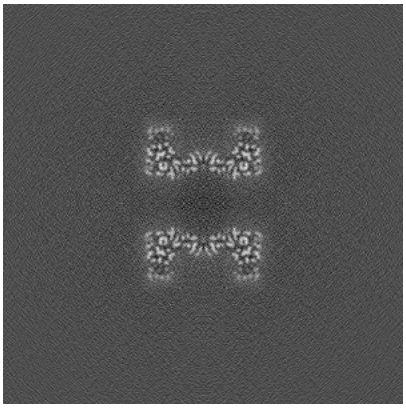


Z Index: 200

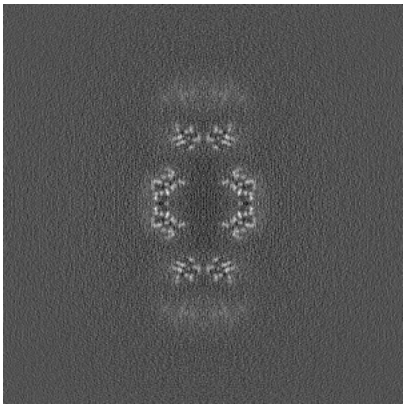
6.2.2 Raw map



X Index: 200



Y Index: 200

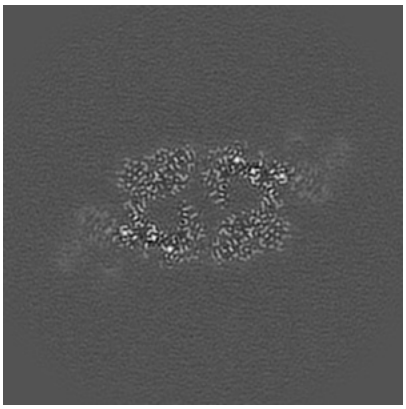


Z Index: 200

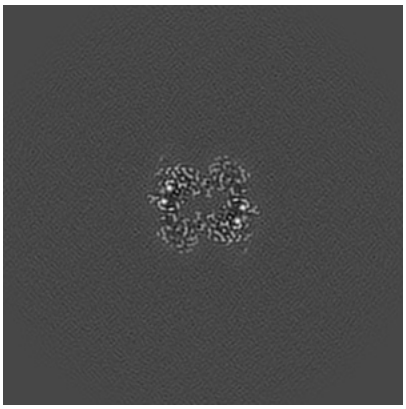
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

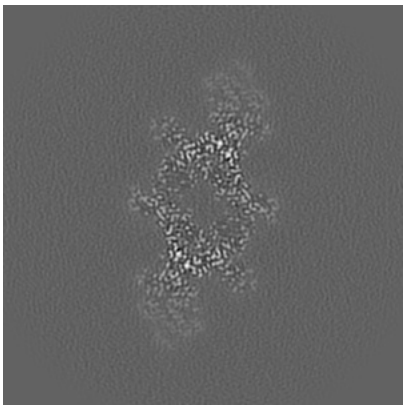
6.3.1 Primary map



X Index: 226

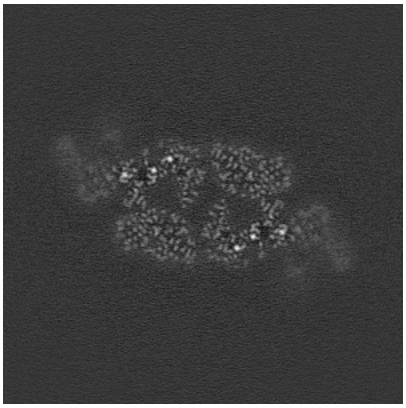


Y Index: 139

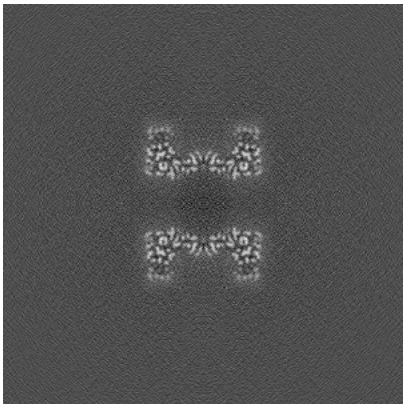


Z Index: 234

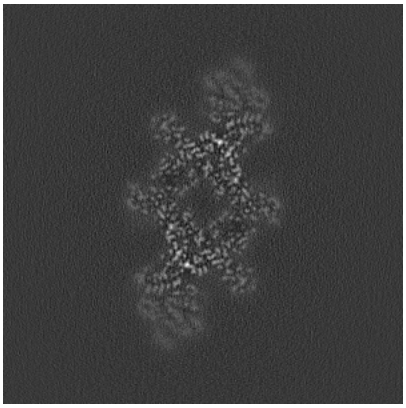
6.3.2 Raw map



X Index: 174



Y Index: 200

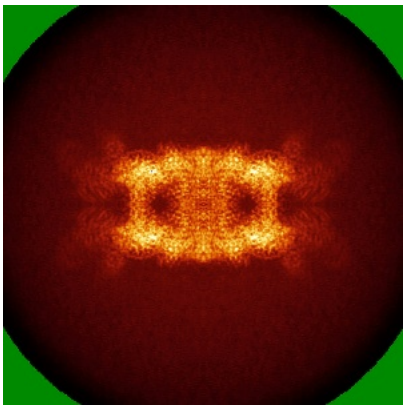


Z Index: 235

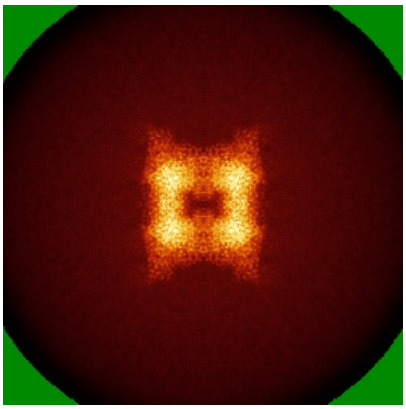
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

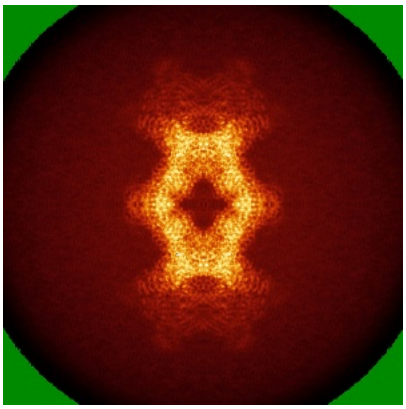
6.4.1 Primary map



X

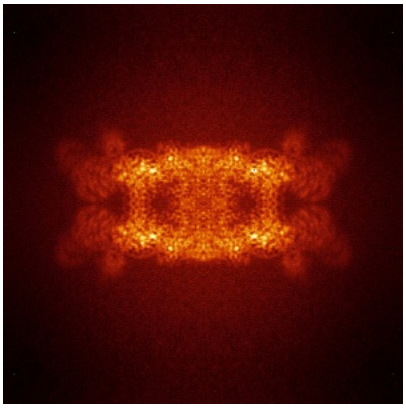


Y

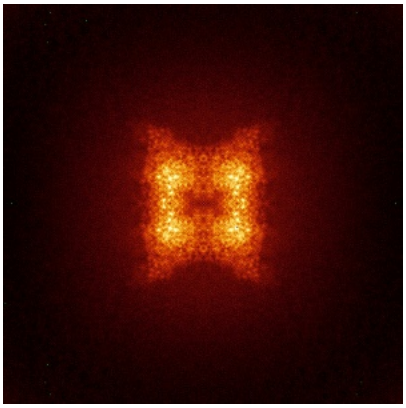


Z

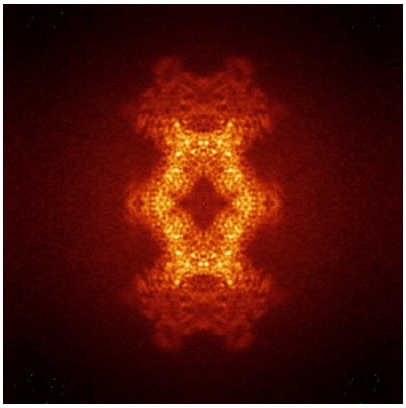
6.4.2 Raw map



X



Y

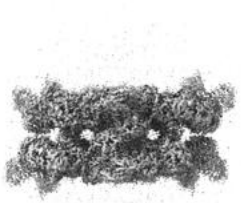


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

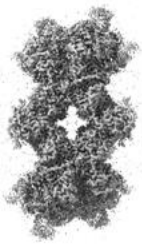
6.5.1 Primary map



X



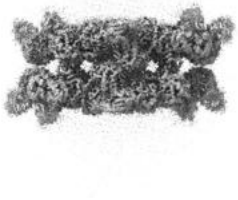
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.164. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

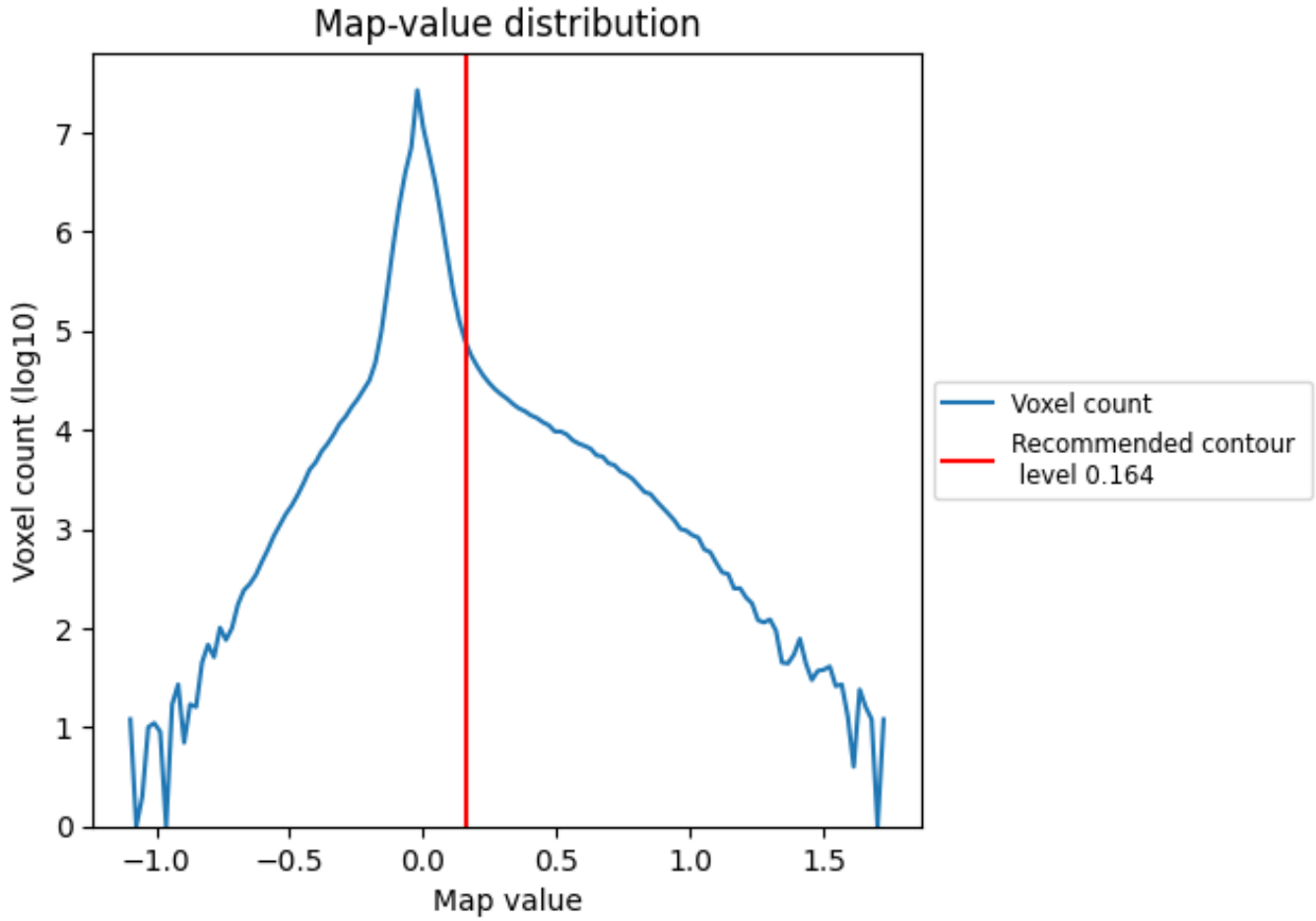
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

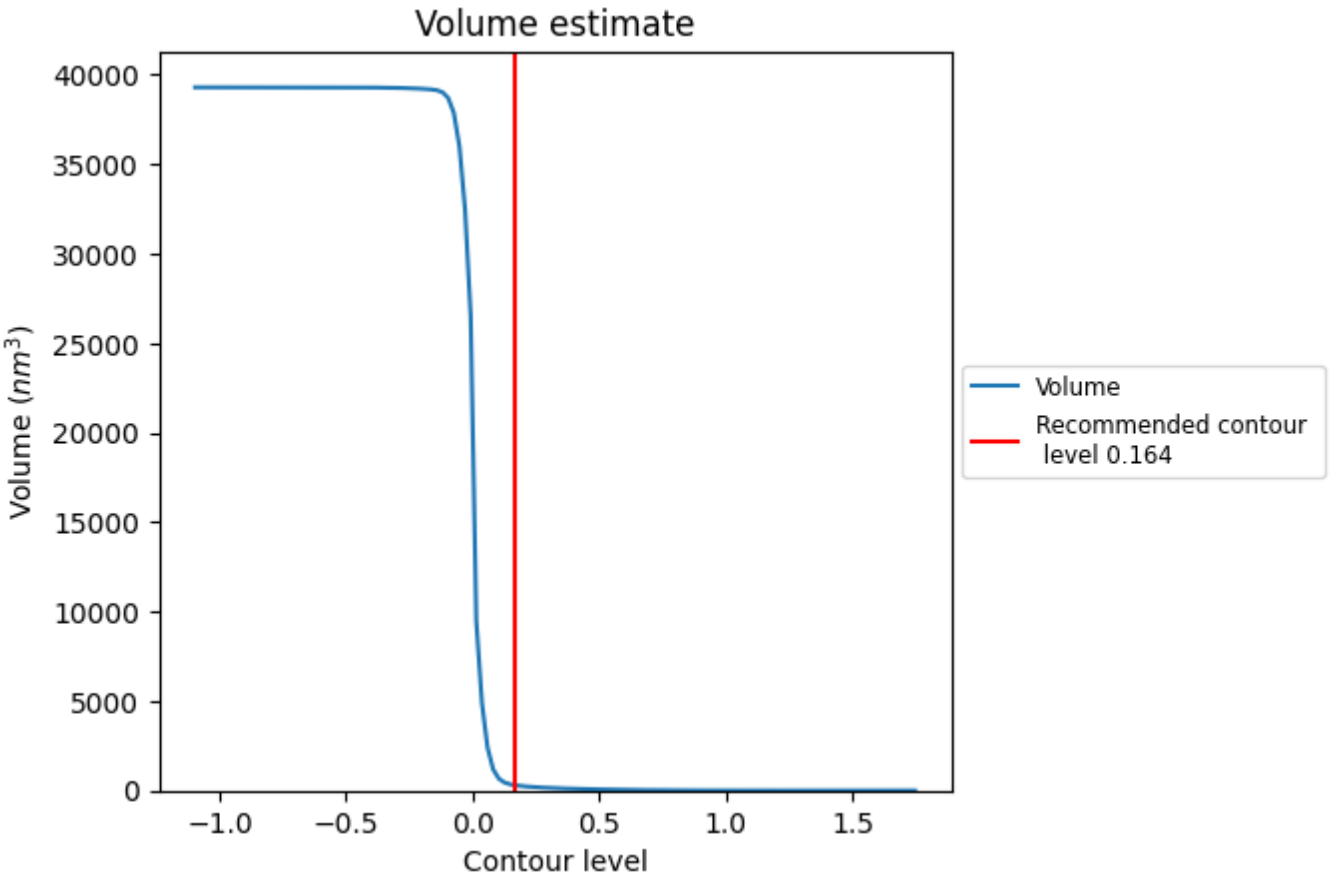
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

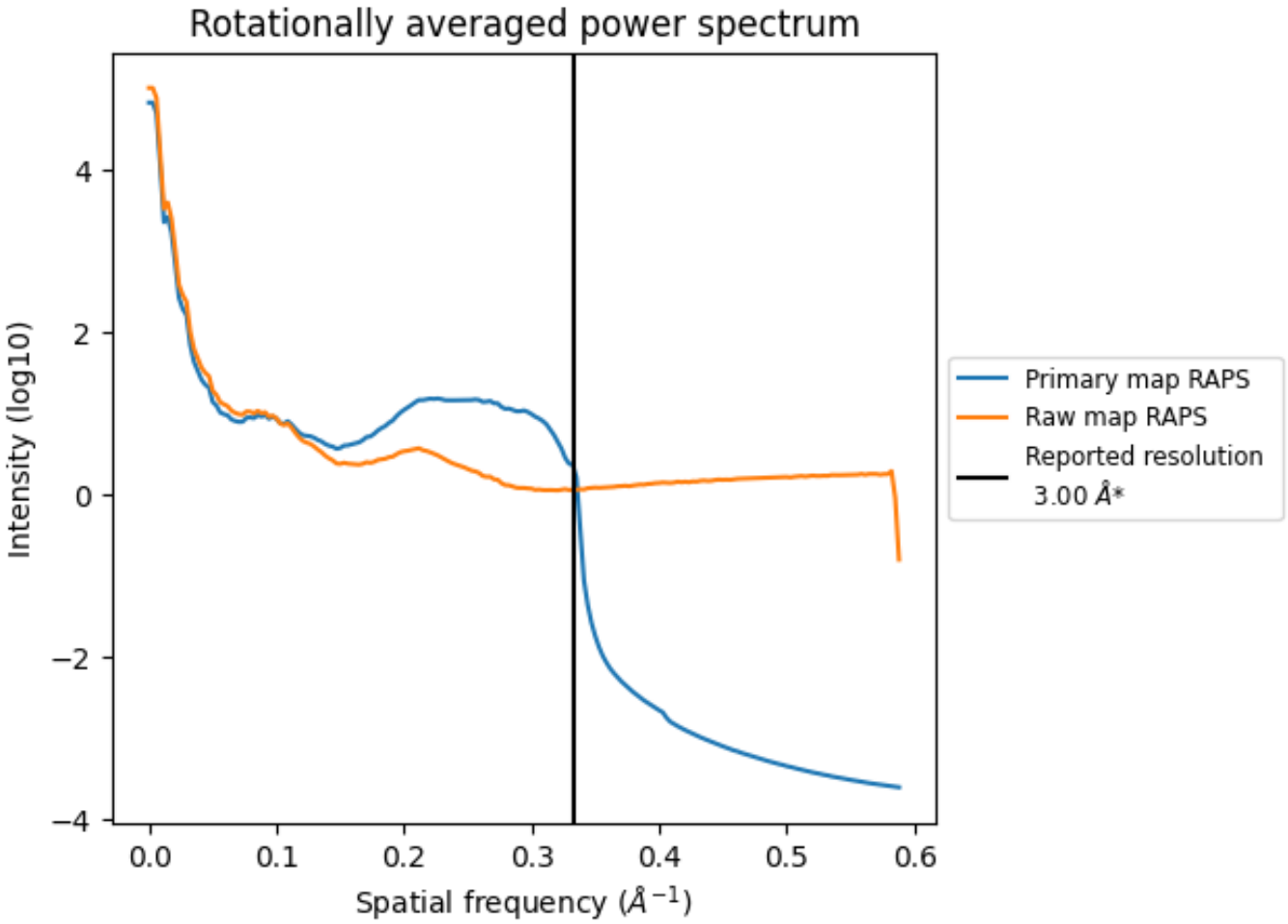
7.2 Volume estimate



The volume at the recommended contour level is 310 nm^3; this corresponds to an approximate mass of 280 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

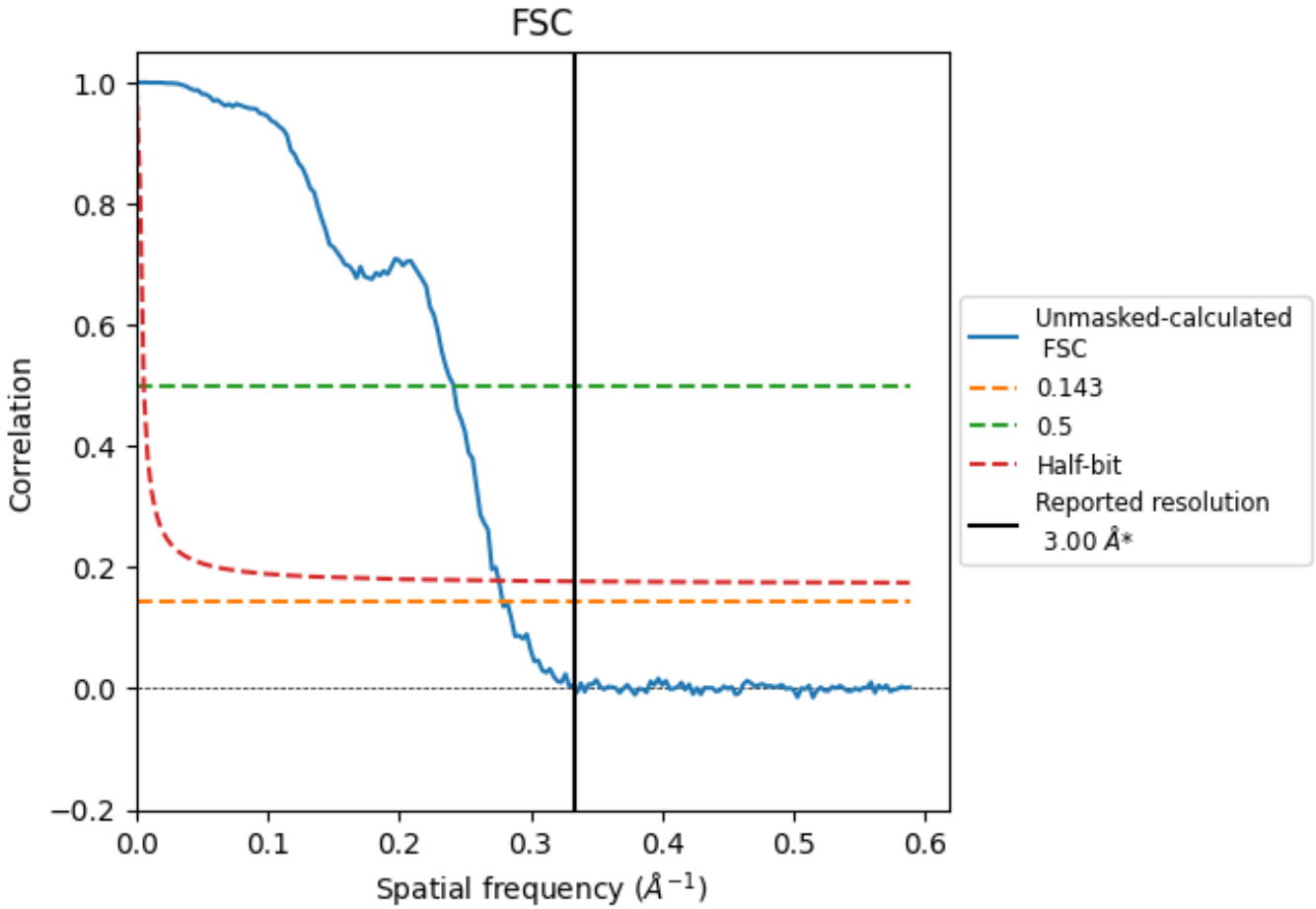


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

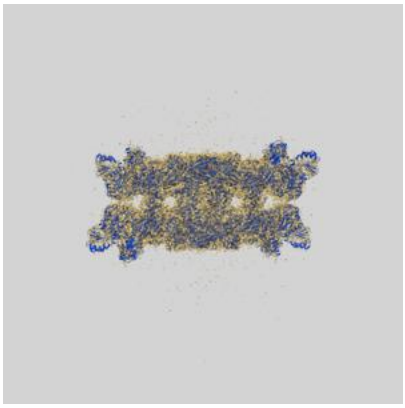
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.59	4.14	3.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.59 differs from the reported value 3.0 by more than 10 %

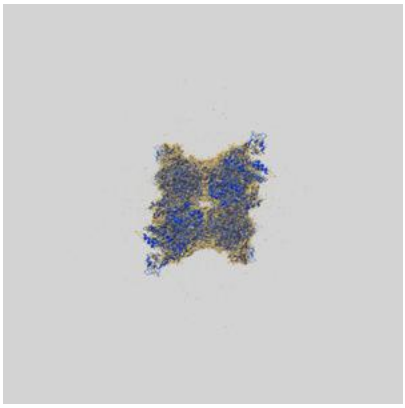
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16878 and PDB model 8OH5. Per-residue inclusion information can be found in section 3 on page 12.

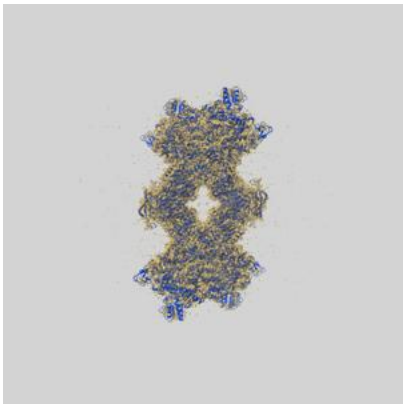
9.1 Map-model overlay



X



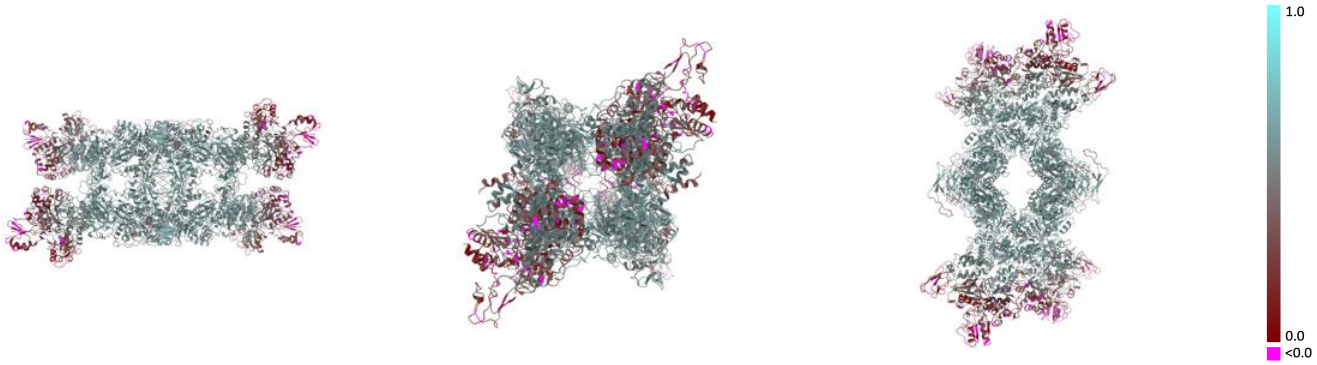
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.164 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

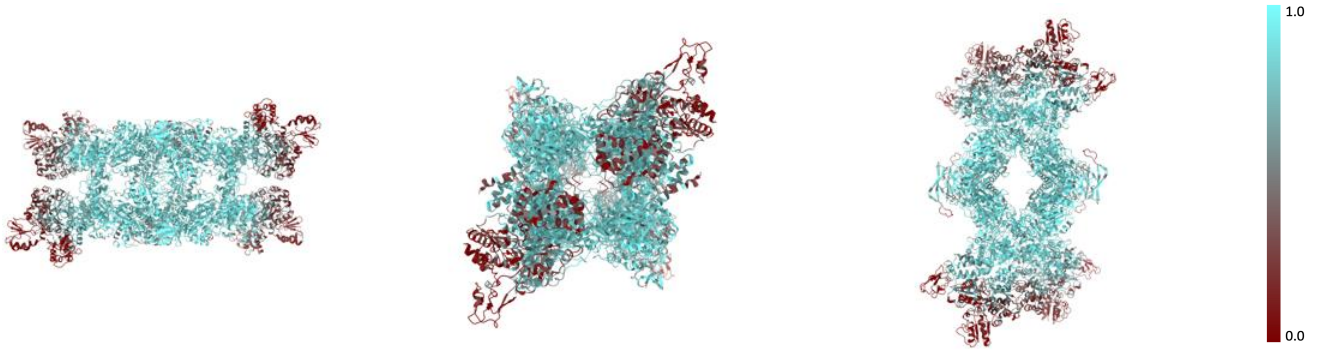
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

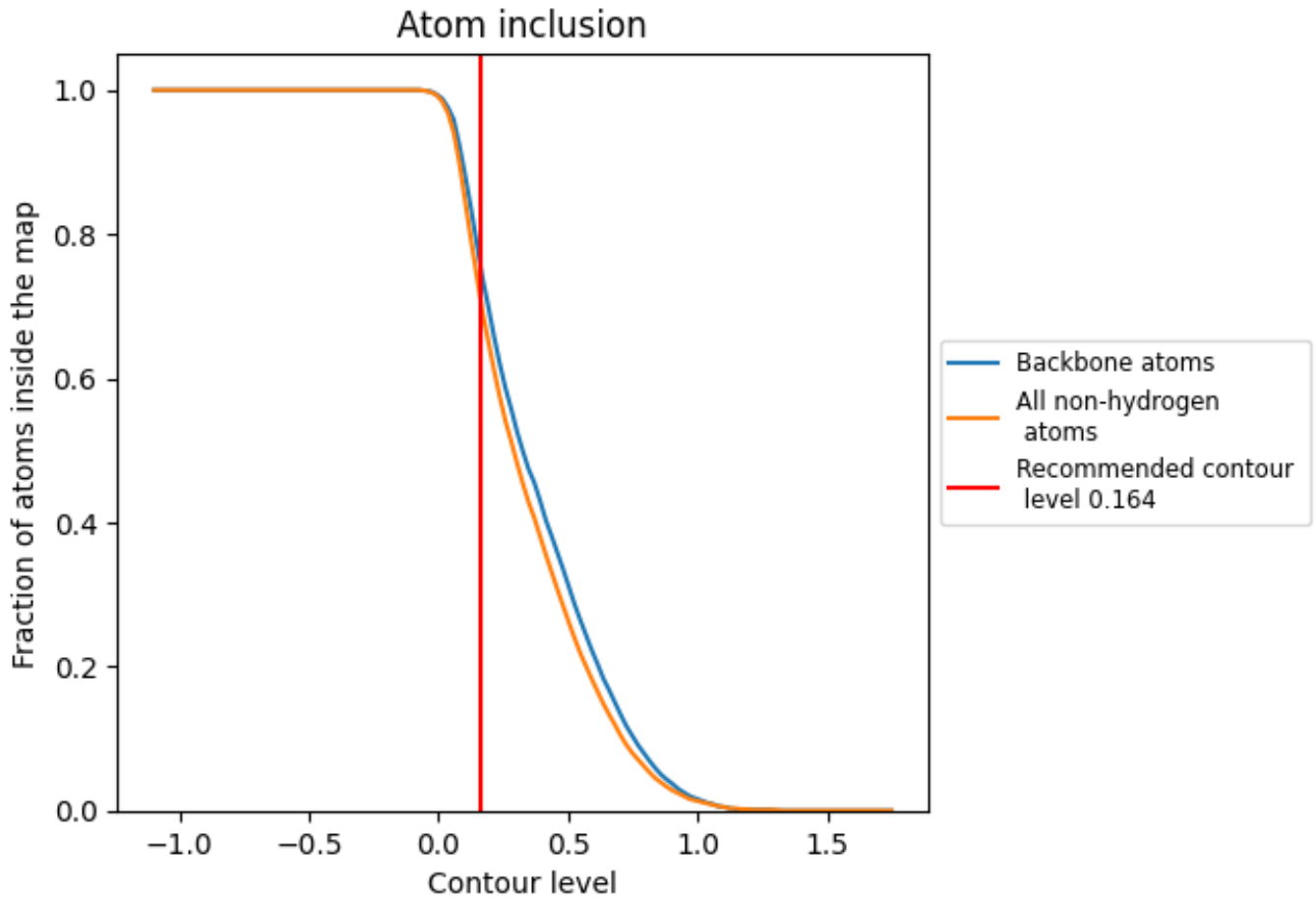
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.164).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.164) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7060	0.4910
A	0.4500	0.3760
B	0.4340	0.3390
C	0.8750	0.5820
D	0.4510	0.3770
E	0.4360	0.3390
F	0.8750	0.5810
G	0.4490	0.3780
H	0.4360	0.3390
I	0.8750	0.5810
J	0.4510	0.3790
K	0.4360	0.3410
L	0.8750	0.5810

